Standard X-ray Diffraction Powder Patterns

Section 11—Data for 70 Substances

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Circular 539

Volume 2, page 30. In column 2, the density of PbO (red) should be 9.334 g/cm^3.

Volume 4, page 60. In the table column 4, the d-spacing 3.36 should be 2.36.

Volume 6, page 60. In the table column 2, the d-spacing 2.75 should be 1.75.

Volume 7, page 29. In the table, the NBS d-spacing 1.426 should be 1.406.

Monograph 25

Section 4, page 31. In the reference 4, the formula should be $KC_6H_4COOH\text{-}COO$.

Section 7, page 2
Section 8, page 3
Section 9, page 3
Section 10, page 3

In each section, the formula for L_p should be:

$$L_p = \frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}$$

Section 8, page 3. The formula for B should be:

$$B = 4\left[\frac{\beta_{11}\beta_{22}\beta_{33}}{a^{*2}b^{*2}c^{*2}}\right]^{\frac{1}{3}}$$

Section 9, page 115. The index entry for ammonium chloroosmate, $(NH_4)_2OsCl_6$, should be Sec. 1m, pg. 6.

Section 10, page 11. In the sample description, line 2, BrF_2 should be BaF_2.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

The following copies may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, Virginia, 22151. Where these publications are identified with a number, it must be used in ordering. They are available in hardcopy or microfiche; the price is not fixed and will be furnished on request.

NBS Publication	Number	NBS Publication	Number
Circular 539, Volume 1	PB 178 902	Monograph 25, Section 1	PB 178 429
Volume 2	PB 178 903	Section 2	PB 178 430
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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 11. --- Data for 70 Substances

by

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Assisted by Johan H. de Groot[2] and Simon J. Carmel

Standard x-ray diffraction patterns are presented for 70 substances. Fifty-two of these patterns represent experimental data and 18 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

Key words: Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the Joint Committee on Powder Diffraction Standards,[3] the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the Joint Committee, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 70 compounds (52 experimental and 18 calculated patterns), and is the twenty-first of the series of "Standard X-ray Diffraction Powder Patterns."[4]

[1,2]Consultant and Research Associates, respectively, of the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards.

[3]Joint Committee on Powder Diffraction Standards, 1601 Park Lane, Swarthmore, Pa. 19081. This Pennsylvania non-profit corporation functions in cooperation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, The Clay Minerals Society, The Institute of Physics, the Mineralogical Association of Canada, the Mineralogical Society of America, The Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Française de Minéralogie et de Cristallographie.

[4]See previous page for other published volumes.

EXPERIMENTAL POWDER PATTERNS

Sample. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory. Appropriate annealing or recrystallization of the sample improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

Optical data, color. A microscopic inspection for phase purity was also made on the non-opaque materials during the refractive index determination. The latter was done by grain-immersion methods in white light, using oils standardized in sodium light, in the refractive index range 1.40 to 2.1 [Hartshorne and Stuart, 1970].

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts [1965].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard (approximately 5 wt. percent tungsten powder). If tungsten lines were found to interfere with lines from the sample, silver was used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used. To avoid errors associated with aberrations at the very top of peaks, the readings of 2θ were taken at positions about 20 percent of the way down from the top, and in the center of the peak width. The internal standard correction for each region was then applied to the measured value of 2θ. We have reported all data as $K\alpha_1$ peaks because the internal standard corrections for all regions were established in terms of the $K\alpha_1$ wavelength.

The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in the table below; the 2θ angles were computed using cell dimensions uncorrected for index of refraction.

Calculated 2θ Angles, CuKα$_1$ λ = 1.54056 Å

hkℓ	W a = 3.16516 Å ±.00004	Ag a = 4.08641 Å ±.00002
110	40.262°	
111		38.112°
200	58.251	44.295
211	73.184	
220	86.996	64.437
310	100.632	
311		77.390
222	114.923	81.533
321	131.171	
400	153.535	97.875
331		110.499
420		114.914
422		134.871
511		156.737

All of our spacing measurements were recorded at 25 ± 1 °C on a diffractometer equipped with a curved lithium fluoride crystal monochromator located between the sample and the Geiger counter. Copper radiation was used and the wavelength Kα$_1$ was taken to be 1.54056 Å [Bearden, 1964].

Structure, lattice constants. The space groups were listed with short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography, Vol. I [1952].

Orthorhombic cell dimensions were arranged according to the Dana convention b>a>c [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary, in order to follow the convention of using a cell with the three shortest edges [Crystal Data, Vol. II, 1973].

A computer program [Evans et al. 1963] assigned hkℓ's and refined the lattice constants. Cell refinement was based only upon $2\theta_{obs}$ values which could be indexed without ambiguity. The program minimized the value $\Sigma(\theta_{obs}-\theta_{calc})^2$. The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Beginning with this issue, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants in earlier publications of this series. In indexing cubic patterns, multiple hkℓ's were not utilized in the refinement or reported. Instead, the single appropriate index having the largest h was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

Densities. These were calculated from the NBS determined lattice constants, the Avogadro number (6.02252×10^{23}), and atomic weights based on carbon 12 [International Union, 1961].

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10 μm, as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (as shown in Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line. At least three patterns for intensity measurements were prepared for each sample to check reproducibility.

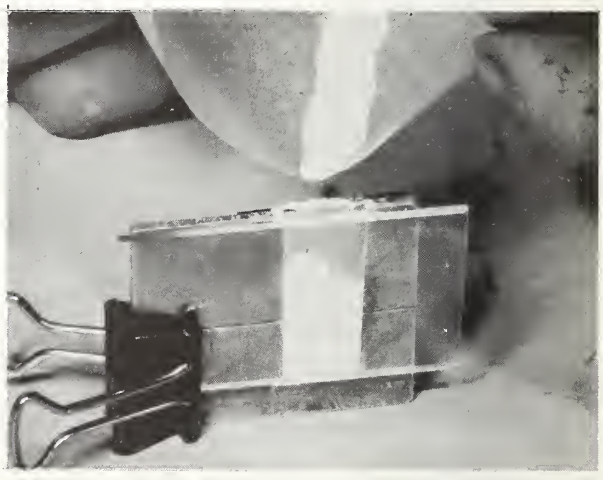

Figure 1

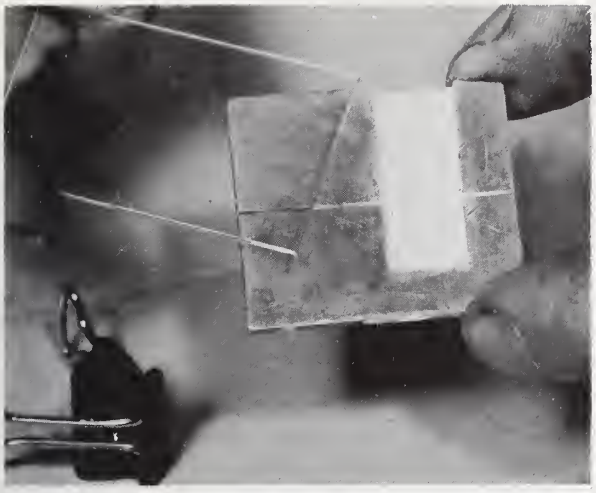

Figure 2

Reference intensity, $I/I_{corundum}$. For reference intensity measurements, α-Al_2O_3 (corundum) was chosen as an internal standard to be mixed 1:1 by weight with the sample. This mixture of two components was mounted in our regular intensity sample holder (see Figures 1 and 2), and the pattern was taken. The reference intensity was then calculated as the direct ratio of the strongest line of the sample to the strongest line of corundum (hexagonal reflection (113)). In a few instances, the strongest line of one of the components coincided with a line of the other. In that case, the second strongest line was measured, and the value for the strongest line was then calculated.

CALCULATED POWDER PATTERNS

Since some substances of interest are not readily available for experimental work, powder patterns were calculated from published crystal structure data. The FORTRAN program used for the computations was developed by Smith [1967] and modified at NBS.

Lattice parameters. Before the computations of the patterns, changes were made as necessary in the lattice constants in order to make then consistent with the revised value of the copper wavelength [Bearden, 1964]; specifically, a published lattice constant in Å was multiplied by 1.00004. Both the altered parameter and the original published value are given. Monoclinic and triclinic lattice constants were transformed if necessary, to follow the convention of using a cell with the 3 shortest edges [Crystal Data, Vol. II, 1973].

Scattering factors. Whenever possible, the same scattering factors were used which the author of the reference article specified. Otherwise, the factors were taken directly from the International Tables for X-ray Crystallography, Vol. III, [1962]. The factors were corrected for dispersion if the author had done so.

Thermal parameters. The computer program used thermal parameter data of only two forms, the isotropic B's or the anisotropic β_{ij}'s in the following expressions:

$$e^{(-B \sin^2\theta)/\lambda^2}$$

or

$$e^{-(h^2\beta_{11}+k^2\beta_{22}+\ell^2\beta_{33}+2hk\beta_{12}+2h\ell\beta_{13}+2k\ell\beta_{23})}.$$

Other thermal parameters were converted to one of these two forms. The isotropic parameters were used directly, if given by the structure reference. In a few of our patterns, anisotropic parameters were also used directly as given by the structure reference; in other work, in place of using given anisotropic parameters, approximately equivalent isotropic values were substituted as defined by:

$$B = 4\left[\frac{\beta_{11}\beta_{22}\beta_{33}}{a^{*2}\, b^{*2}\, c^{*2}}\right]^{\frac{1}{3}}$$

Integrated intensities. Intensity calculations were based on the copper $K\alpha_1$ wavelength, 1.54056 Å, determined by Bearden [1964]. The integrated intensities were computed from formula (1):

(1) $$I = F^2 \,(Lp)\,(FAC)$$

where F is the standard structure factor

FAC is the powder multiplicity

$$Lp = \frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}$$

The intensities were scaled to the strongest line which was assigned a value of 100. Reflections were not reported which had scaled intensities of 0.7 or less.

Scale factor. For each compound, this factor multiplied by the reported integrated intensities will reproduce the unscaled intensities which were derived using formula (1).

Peak intensities. The integrated intensities can be transformed to a Cauchy profile with an appropriate variable half-width designated to simulate a diffractometer tracing [Smith, 1967]. The value of the half-width was chosen as 0.075° at 40° (2θ, $CuK\alpha_1$). Then the intensities were summed for the overlapping peak profiles, and the resulting new peak intensities were scaled to the strongest peak height which was assigned a value of 100. Reflections were not reported which had scaled peak heights of 0.7 or less. Adjacent peaks with nearly equal 2θ values usually cannot be experimentally resolved; therefore one composite peak was calculated in such instances. The 2θ angle of this peak was assigned the $hk\ell$ of the reflection having the greatest integrated intensity; a plus sign (+) was used to indicate additional $hk\ell$'s.

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Palache, C., Berman, H. and Frondel, C. (1944). Dana's System of Mineralogy (John Wiley and Sons, New York, 7th Ed.), I, 6.

Smith, D.K. (1967). A Revised Program for Calculating Powder Diffraction Patterns,UCRL 50264, University of California, Lawrence Radiation Laboratory, Livermore, Calif. 94551.

Aluminum bismuth oxide, $Al_4Bi_2O_9$

Sample

The sample was prepared by heating a 2:1 mixture of αAl_2O_3 and Bi_2O_3 at 1000 °C. This was followed by grinding and reheating.

Color

Pale yellow

Structure

Orthorhombic, Pbam (55), Z=2, isostructural with $Bi_2Ga_4O_9$. The structure was determined by Eckerlin and Liebertz [1965].

NBS lattice constants:
a = 7.719(1)Å
b = 8.109(1)
c = 5.6919(8)

Density

(calculated) 6.244 g/cm³

Reference intensity

$I/I_{corundum}$ = 3.1

Additional patterns

1. PDF card 23-1006 [Surnina and Litvin, 1970].

References

Eckerlin, P. and Liebertz, J. (1965). Naturwissenschaften **52**, 540.

Surnina, V.S. and Litvin, B.N. (1970). Soviet Phys. Cryst. English Transl. **15**, 527.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.68	75	001	15.58
4.055	12	020	21.90
3.989	5	111	22.27
3.862	10	200	23.01
3.591	35	120	24.77
3.485	25	210	25.54
3.301	19	021	26.99
3.192	20	201	27.93
3.034	100	121	29.41
2.971	85	211	30.05
2.846	30	002	31.41
2.795	12	220	32.00
2.551	15	130	35.15
2.537	14	112	35.35
2.510	3	221	35.75
2.453	9	310	36.60
2.328	16	022,131	38.65
2.290	14	202	39.31
2.252	11	311	40.01
2.230	12	122	40.42
2.204	35	212	40.91
2.028	1	321,040	44.64
1.994	1	222	45.44
1.961	12	140	46.26
1.930	3	400	47.05
1.908	2	041	47.61
1.898	10	132,003	47.88
1.878	7	410	48.44
1.864	15	330	48.83
1.857	16	312	49.02
1.854	25	141	49.10
1.827	1	401	49.87
1.795	3	240	50.82
1.783	16	411	51.18
1.771	17	331	51.55
1.743	3	420	52.46
1.726	1	322	53.00
1.719	2	023	53.25
1.703	2	203	53.77
1.677	14	123	54.69
1.666	13	213,421	55.07
1.652	5	042	55.60
1.615	7	142	56.98
1.597	5	402	57.66
1.567	9	412	58.87
1.559	25	332	59.21
1.528	1	151	60.54
1.5222	2	133	60.80
1.5004	2	313	61.78
1.4954	2	250	61.98
1.4655	1	511	63.42
1.4465	6	251	64.35
1.4233	5	004	65.53
1.3989	6	521	66.82
1.3865	3	152	67.50
1.3722	2	350	68.30
1.3638	5	143	68.78

Aluminum nitrate hydrate, $Al(NO_3)_3 \cdot 9H_2O$

Sample

The sample was prepared by slow evaporation of an aqueous solution of $Al(NO_3)_3$. The crystals were filtered out and washed with ethyl alcohol.

Color

Colorless

Optical data

Biaxial (-), $N_\alpha = 1.401$, $N_\beta = 1.514$, $N_\gamma = 1.525$; $2V \cong 25°$.

Structure

Monoclinic, $P2_1/c$ (14), Z=4, isostructural with $Cr(NO_3)_3 \cdot 9H_2O$ [Kannan and Viswamitra, 1965].

NBS lattice constants:

a = 13.847(8)Å
b = 9.617(2)
c = 10.908(5)
β = 95.68(2)°

Density

(calculated) 1.724 g/cm^3

Reference intensity

$I/I_{corundum}$ 0.5

Additional patterns

1. PDF card 1-435 [Hanawalt et al., 1938]
2. PDF card 12-472 [Aluminium Lab. Ltd.,Kingston Canada].

References

Hanawalt, J.D., Rinn, H.W., and Frevel, L.K.(1938) Ind. Eng. Chem. Anal. Ed. 10, 457.

Kannan, K. K. and Viswamitra, M. A. (1965). Acta Cryst. 19, 151.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
7.87	1	110	11.24
7.20	12	011	12.29
6.55	70	$\bar{1}11$	13.51
6.21	60	111	14.26
5.60	14	210	15.81
5.22	6	$\bar{1}02$	16.97
4.89	18	102	18.13
4.82	25	211,020	18.41
4.729	4	012	18.75
4.595	4	$\bar{1}12$,300	19.30
4.539	15	$\bar{1}20$	19.54
4.487	45	$\bar{2}02$	19.77
4.362	3	$\bar{1}12$	20.34
4.231	2	$\bar{1}21$	20.98
4.143	10	310,121	21.43
4.074	60	$\bar{2}02$	21.80
3.994	45	$\bar{3}11$	22.24
3.943	50	220	22.53
3.762	30	311	23.63
3.639	12	221	24.44
3.599	65	022	24.72
3.541	6	$\bar{1}22$	25.13
3.449	9	$\bar{3}12$,400	25.81
3.426	12	122	25.99
3.387	6	013	26.29
3.278	16	$\bar{2}22$	27.18
3.244	35	410,$\bar{3}21$	27.47
3.219	19	113	27.69
3.123	20	130	28.56
3.112	20	321	28.66
3.074	12	031	29.02
3.049	20	$\bar{4}02$	29.27
3.017	100	$\bar{1}31$	29.58
2.982	45	131	29.93
2.907	35	230,$\bar{4}12$	30.73
2.878	7	$\bar{1}23$	31.05
2.854	5	$\bar{3}13$	31.32
2.835	4	$\bar{2}31$	31.53
2.788	3	402,123	32.08
2.779	7	231	32.18
2.761	18	032	32.40
2.680	6	132	33.41
2.615	20	$\bar{2}04$,104,+	34.26
2.609	30	014,$\bar{2}32$,+	34.34
2.590	50	$\bar{3}31$	34.60
2.538	16	$\bar{3}23$	35.33
2.522	35	331,114,+	35.57
2.446	3	$\bar{3}04$,204	36.71
2.422	2	$\bar{3}32$	37.09
2.399	6	033	37.45
2.393	4	$\bar{5}20$,$\bar{1}33$	37.56
2.369	40	$\bar{3}14$,140,+	37.95
2.363	25	$\bar{1}24$,024,+	38.05
2.348	30	041,430	38.31
2.326	4	$\bar{4}31$	38.68
2.307	12	$\bar{4}23$,141	39.01
2.301	14	$\bar{2}24$,600,+	39.16
2.271	16	240	39.65
2.263	8	$\bar{4}31$,$\bar{5}22$	39.80
2.242	10	$\bar{4}04$,$\bar{5}13$,+	40.19
2.210	2	$\bar{4}32$,241	40.79
2.184	16	$\bar{1}42$,$\bar{4}14$,+	41.30

Aluminum tungsten oxide, $Al_2(WO_4)_3$

Sample

The sample was prepared by adding $NaWO_4$ solution to one of $AlCl_3$ and heating the precipitate two hours at 800 °C and 15 minutes at 900 °C.

Color

Colorless

Structure

Orthorhombic, Pnca (60), Z=2, isostructural with other tungstates and molybdates of the smaller trivalent rare-earth elements such as $Gd_2(WO_4)_3$ [Craig and Stephenson, 1968].

NBS lattice constants:

a = 9.139(2) Å
b = 12.596(2)
c = 9.060(2)

Density

(calculated) 2.539 g/cm^3

Reference intensity

$I/I_{corundum} = 2.3$

Additional patterns

1. PDF card 18-72 [Waring, 1965] (incorrectly called $2Al_2O_3 \cdot 5WO_3$)

References

Craig, D. C. and Stephenson, N. C. (1968). Acta Cryst. B24, 1250.

Waring, J. (1965). J. Am. Ceram. Soc. 48, 493.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
6.30	11	020	14.04
5.73	13	111	15.46
4.53	11	002	19.59
4.50	6	121	19.73
4.296	35	210	20.66
4.059	40	102	21.88
3.877	50	211	22.92
3.867	45	112	22.98
3.810	100	031	23.33
3.697	16	220	24.05
3.676	7	022	24.19
3.519	25	131	25.29
3.422	50	221	26.02
3.219	15	202	27.69
3.147	12	040	28.34
3.115	4	212	28.63
3.090	6	230	28.87
2.933	19	013	30.45
2.926	10	231	30.53
2.865	13	222	31.19
2.828	6	141	31.61
2.816	9	311	31.75
2.624	7	321	34.14
2.610	16	123	34.33
2.593	7	240	34.56
2.555	2	232	35.10
2.528	7	302	35.48
2.493	8	241	36.00
2.488	9	142	36.07
2.480	7	312	36.19
2.471	6	213	36.32
2.429	5	051	36.98
2.380	5	331	37.76
2.368	19	133	37.97
2.346	3	322,151	38.34
2.340	4	223	38.45
2.285	2	400	39.40
2.265	3	004	39.77
2.252	7	242	40.01
2.206	11	250	40.87
2.182	17	411	41.35
2.166	6	114,332	41.67
2.161	5	233	41.77
2.142	10	251,152	42.15
2.132	5	024	42.35
2.114	5	313	42.73
2.100	13	060	43.03
2.076	1	124	43.56
2.030	3	323,204	44.61
2.004	9	214	45.21
1.984	3	252	45.70
1.972	9	342	45.99
1.959	2	431	46.30
1.941	6	422	46.77
1.935	5	053	46.92
1.907	6	260	47.66
1.8926	3	153	48.03
1.8650	13	162	48.79
1.8490	13	440	49.24
1.8385	9	044	49.54
1.8271	3	234	49.87
1.7987	2	314	50.73
1.7931	5	015	50.88
1.7833	5	352	51.18

Ammonium copper fluoride, NH_4CuF_3

Sample

The sample was prepared by the reaction of Cu and Br in methanol; the product was added to a saturated methanol solution of NH_4HF_2. The precipitate was filtered, and washed with methanol and ether. The sample was somewhat hygroscopic.

Color

Greenish white

Structure

Tetragonal, P4mm (99), Z=2, similar to $KCuF_3$, distorted perovskite. Crockett and Haendler [1960] gave a larger cell related to ours as $a \cong a\sqrt{2}$ and $c \cong 2c$. We found no lines which required the larger cell.

NBS lattice constants:

a = 6.0828(4)Å
c = 3.8915(4)

Density (calculated) 3.196 g/cm³

Reference intensity $I/I_{corundum} = 2.4$

Additional patterns

1. PDF card 22-41 [Clavan, 1969, Pennwalt Corp. King of Prussia, Penna.]

References

Crockett, D.S. and Haendler, H.M.(1960). J. Am. Chem. Soc. 82, 4158.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.300	100	110	20.64
3.889	35	001	22.85
3.041	35	200	29.35
2.885	55	111	30.97
2.719	4	210	32.92
2.395	3	201	37.52
2.230	4	211	40.42
2.150	50	220	41.98
1.946	19	002	46.64
1.924	18	310	47.20
1.882	15	221	48.31
1.773	15	112	51.50
1.725	14	311	53.05
1.640	8	202	56.04
1.5478	2	321	59.69
1.5208	9	400	60.86
1.4753	3	410	62.95
1.4429	17	222	64.53
1.4336	5	330	65.00
1.4166	5	401	65.88
1.3681	9	312	68.53
1.3601	5	420	68.99
1.3453	4	331	69.86
1.2970	2	003	72.87
1.2419	4	113	76.67
1.1983	6	402	80.00
1.1930	5	203,510	80.43
1.1755	2	412	81.88
1.1542	5	332	83.73
1.1407	5	511	84.95
1.1146	4	422	87.43
1.1109	3	223	87.80
1.0756	4	313,440	91.47
1.0169	4	512	98.48

Ammonium formate, $HCOONH_4$

Sample

The sample was obtained from the K and K Laboratories, Inc., Jamaica, N.Y. The material was somewhat hygroscopic.

Color

Colorless

Structure

Monoclinic , Pc (7), Z=2. The structure was determined by Nahringbauer [1968].

NBS lattice constants

a = 3.8202(5)Å
b = 4.6816(6)
c = 9.118(1)
β = 91.12(1)°

Density

(calculated) 1.284 g/cm^3

Reference intensity

$I/I_{corundum}$ = 1.5

Additional patterns

1. PDF card 14-756 [Hanawalt et al., 1938]

References

Hanawalt, J.D., Rinn,H.W.,and Frevel, L.K.(1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

Nahringbauer, I. (1968). Acta Cryst. B24,565.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ (°)
4.555	55	002	19.47
4.164	65	011	21.32
3.819	10	100	23.27
3.266	14	012	27.28
2.954	100	110,102	30.23
2.898	5	$\bar{1}02$	30.83
2.826	30	$\bar{1}11$	31.63
2.802	6	111	31.91
2.550	9	013	35.17
2.500	10	$\bar{1}12$	35.89
2.466	9	112	36.41
2.340	8	020	38.43
2.279	13	004	39.51
2.267	11	021	39.73
2.137	2	$\bar{1}13$	42.26
2.105	1	113	42.92
2.083	4	022	43.41
2.049	7	014	44.16
1.996	1	120	45.39
1.974	4	$\bar{1}04$	45.93
1.955	1	$\bar{1}21$	46.42
1.945	2	121	46.66
1.941	1	104	46.76
1.9095	1	200	47.58
1.8546	4	023	49.08
1.8350	1	$\bar{1}22$	49.64
1.8192	2	$\bar{1}14$	50.10
1.7932	<1	114	50.88
1.7733	2	$\bar{2}02$	51.49
1.7685	2	210	51.64
1.7490	1	202	52.26
1.7419	1	$\bar{2}11$	52.49
1.7296	1	211	52.89
1.6990	2	015	53.92
1.6758	2	$\bar{1}23$	54.73
1.6598	2	123,$\bar{2}12$	55.30
1.6335	<1	105,024	56.27
1.5635	2	$\bar{1}15$	59.03
1.5406	2	$\bar{2}13$	60.00
1.5380	2	031	60.11
1.5193	1	006	60.93
1.5085	1	$\bar{1}24$	61.41
1.4938	<1	124	62.08
1.4801	<1	220	62.72
1.4767	1	032	62.88
1.4646	1	$\bar{2}21$	63.46
1.4574	1	221	63.81
1.4451	1	016,130	64.42
1.4283	2	$\bar{1}31$	65.27
1.4246	2	131	65.46

Sample

Chlorine was bubbled through a saturated solution of $PbCl_2$ in concentrated HCl. Then a saturated solution of NH_4Cl in concentrated HCl was added. The precipitate formed was filtered without washing.

Color

Brilliant green yellow

Structure

Cubic, Fm3m (225), Z=4, isostructural with K_2PtCl_6. The structure was determined by Wyckoff and Dennis [1926].

NBS lattice constant:
a = 10.1609(3) Å

Density

(calculated) 2.887 g/cm^3

Reference intensity

$I/I_{corundum}$ = 3.6

Additional patterns

1. PDF card 2-0139 [Wyckoff and Dennis, 1926].

Reference

Wyckoff, R. W. G. and Dennis, L. M. (1926). Am. J. Sci. 12, 503.

Internal standard W, a = 3.16516 Å

$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.866	100	111	15.09
5.081	45	200	17.44
3.593	20	220	24.76
3.061	45	311	29.15
2.933	1	222	30.45
2.540	25	400	35.31
2.332	18	331	38.57
2.272	25	420	39.63
2.074	9	422	43.61
1.955	14	511	46.41
1.796	15	440	50.78
1.718	12	531	53.29
1.693	10	600	54.11
1.607	2	620	57.28
1.5495	4	533	59.62
1.4667	3	444	63.36
1.4229	4	711	65.55
1.4090	2	640	66.28
1.3577	2	642	69.13
1.3227	4	731	71.23
1.2701	<1	800	74.67
1.2415	1	733	76.70
1.2324	3	820	77.37
1.1976	1	822	80.06
1.1733	2	751	82.07
1.1359	2	840	85.39
1.1152	2	911	87.37
1.1087	2	842	88.02
1.0829	<1	664	90.68
1.0652	1	931	92.63
1.0369	1	844	95.95
1.0211	2	933	97.94
1.0161	1	10·0·0	98.59
0.9964	1	10·2·0	101.25
0.9823	1	951	103.28

Ammonium manganese chloride hydrate, $(NH_4)_2MnCl_4 \cdot 2H_2O$

Sample

The sample was prepared by slow evaporation at room temperature of an aqueous solution containing 2 grams NH_4Cl and 3.6 grams $MnCl_2 \cdot 4H_2O$. The first crystals formed were used. The method follows the phase study of the NH_4Cl-$MnCl_2$-H_2O system by Clendinnen and Rivett [1921].

Color

Pinkish white

Structure

Tetragonal, $P4_2/mnm$ (136), Z=2, isostructural with $(NH_4)_2CuCl_4 \cdot 2H_2O$ [Greenberg and Walden, 1940]. The structure of $(NH_4)_2CuCl_4 \cdot 2H_2O$ was determined by Hendricks and Dickerson [1927] and refined by Chrobak, [1934]. Greenberg and Walden [1940] found $(NH_4)_2MnCl_4 \cdot 2H_2O$ to have a solid solution relation with $(NH_4)_6MnCl_8 \cdot 2H_2O$.

NBS lattice constants:
a = 7.589(1)Å
c = 8.143(2)

Density

(calculated) 1.904 g/cm^3

Reference intensity

$I/I_{corundum} = 1.4$

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.552	35	101	15.95
5.365	15	110	16.51
4.073	35	002	21.80
3.797	6	200	23.41
3.244	8	112	27.47
3.131	8	211	28.48
2.776	100	202	32.22
2.684	90	220	33.36
2.557	8	103	35.06
2.401	4	310	37.43
2.240	25	222	40.22
2.120	5	213	42.61
2.067	1	312	43.76
2.038	19	321	44.41
1.898	16	400	47.89
1.798	3	313	50.72
1.7938	5	204	50.86
1.7194	8	402	53.23
1.6629	4	323	55.19
1.6213	17	224	56.73
1.5660	9	422	58.93
1.5231	2	413	60.76
1.4923	2	431	62.15
1.3877	8	521,404	67.43

References

Chrobak, L. (1934). Z. Krist. **88**, 35.
Clendinnen, F.W.J. and Rivett, A.C.D. (1921). J. Chem. Soc. **119**, 1329.
Greenberg, A.L. and Walden, G. H. Jr. (1940). J. Chem. Phys. **8**, 645.
Hendricks, S.B. and Dickerson, R.G. (1927). J.Am. Chem. Soc. **49**, 2149.

Additional patterns

1. PDF card 2-844 [Greenberg and Walden, 1940].

Barium hydroxide phosphate, $Ba_5(OH)(PO_4)_3$

Sample

The sample was prepared by heating $Ba(OH)_2$ and $(NH_4)_2HPO_4$ together in a molar ratio of 5 : 3. After heating at 300 °C, the material was pelletized and reheated at 600 °C for one hour, at 900 °C for one hour, and at 1100 °C for one half hour.

Color

Colorless

Structure

Hexagonal, $P6_3/m$ (176), Z=2, isostructural with calcium and lead hydroxyapatites [Klement and Dihn, 1938]. The structure of $Ca_5(OH)(PO_4)_3$ was refined by Posner et al. [1958].

NBS lattice constants:
a = 10.185(1)Å
c = 7.729(1)

Density

(calculated) 4.728 g/cm^3

Reference intensity

$I/I_{corundum} = 2.5$

Additional patterns

1. PDF card 1-811 [Hanawalt et al., 1938]
2. PDF card 3-578 [Klement and Dihn, 1938]

References

Hanawalt, J.D., Rinn, H.W.,and Frevel, L.K.(1938). Ind. Eng. Chem. Anal. Ed. **10**, 457.

Klement, R. and Dihn, P. (1938). Z. anorg. u. allgem. Chem. 240, 40.

Posner, A.S., Perloff, A., and Diorio, A.F.(1958). Acta Cryst. **11**, 308.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.10	3	110	17.37
4.410	25	200	20.12
4.255	19	111	20.86
3.869	12	002	22.97
3.829	1	201	23.21
3.541	30	102	25.13
3.334	35	210	26.72
3.079	100	112	28.98
3.062	100	211	29.14
2.940	50	300	30.38
2.908	4	202	30.72
2.546	2	220	35.22
2.447	8	310	36.70
2.338	5	302	38.47
2.334	2	311	38.54
2.299	11	113	39.15
2.225	2	203	40.50
2.205	3	400	40.90
2.127	30	222	42.47
2.067	25	312	43.76
2.038	30	213	44.41
2.023	6	320	44.77
1.958	17	321	46.34
1.932	12	004	47.00
1.925	20	410	47.18
1.915	25	402	47.43
1.868	1	411	48.70
1.807	1	114	50.45
1.792	<1	322	50.91
1.775	1	313	51.45
1.769	3	204	51.62
1.7230	3	412	53.11
1.6979	<1	330	53.96
1.6721	10	214	54.86
1.6671	8	420	55.04
1.6582	3	331	55.36
1.6290	1	421	56.44
1.6143	8	304	57.00
1.6048	5	502	57.37
1.5913	8	323	57.90

Sample

The sample was prepared by melting an equimolar mixture of $BaCl_2$ and $PbCl_2$. It was then ground and heated for 18 hours, at 400 °C, in a sealed glass tube. This was repeated twice.

Color

Colorless

Structure

Orthorhombic, Pnam (62), Z = 2; $BaCl_2$ and $PbCl_2$ form a complete solid solution series [Calingaert et al., 1949]. The structure of $BaCl_2$ was determined by Döll and Klemm [1939] and refined by Brackett et al. [1963] and Sahl [1963].

NBS lattice constant:

a = 7.765(2)Å
b = 9.246(2)
c = 4.658(1)

Density

(calculated) 4.829 g/cm³

Reference intensity

$I/I_{corundum} = 2.8$

References

Brackett, E. B., Brackett, T. E., and Sass, R. L. (1963). J. Phys. Chem. 67, 2132.

Calingaert, G., Lamb, F. W., and Meyer, F. (1949). J. Am. Chem. Soc. 71, 3712.

Döll, W. and Klemm, W. (1939). Z. anorg. u. allgem. Chem. **241**, 239.

Sahl, K. (1963). Beitr. Mineral. Petrog. 9, 111.

Internal standard W, a = 3.16516 Å

$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ (°)
4.62	11	020	19.20
4.16	40	011	21.35
3.97	95	120	22.40
3.885	55	200	22.87
3.664	100	111	24.27
3.020	13	121	29.55
2.981	14	201	29.95
2.972	20	220	30.04
2.866	11	130	31.18
2.838	80	211	31.50
2.572	50	031	34.86
2.508	4	221	35.77
2.440	12	131	36.80
2.415	5	230	37.20
2.331	30	002	38.60
2.311	19	040	38.94
2.259	35	320	39.87
2.215	7	140	40.70
2.197	35	311	41.05
2.142	40	231	42.15
2.081	2	022	43.45
2.009	20	122	45.08
1.997	17	202	45.38
1.986	11	240	45.63
1.941	7	400	46.76
1.833	3	222	49.71
1.759	2	411	51.94
1.678	10	151	54.64
1.675	7	232	54.76
1.642	7	430	55.96
1.6216	15	322	56.72
1.6053	3	142	57.35
1.5720	<1	251	58.68
1.5492	4	431	59.63
1.5110	6	242	61.30
1.5023	5	113	61.69
1.4910	5	402	62.21
1.4869	5	440	62.40
1.4556	7	511	63.90
1.4318	8	351	65.09

Sample

The sample was specially purified material from Mallinckrodt Chemical Works, New York.

Major impurities

0.001–0.01% each: Al, Na, and Sr.

Color

Colorless

Optical data

Isotropic, N = 1.571

Structure

Cubic, $P2_13$ (198), Z = 4, isostructural with $Sr(NO_3)_2$. The structure was determined by Birnstock [1967]. Previously the space group of $Ba(NO_3)_2$ was considered to be Pa3 (205).

NBS lattice constant:
a = 8.1184(2)Å

Density

(calculated) 3.244 g/cm^3

Reference intensity

$I/I_{corundum}$ = 4.5

Additional patterns

1. PDF card 4-773 [Swanson and Tatge, 1953]

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.689	100	111	18.91
4.062	35	200	21.86
3.633	14	210	24.48
3.318	10	211	26.85
2.870	30	220	31.14
2.447	75	311	36.69
2.344	45	222	38.37
2.170	<1	321	41.59
2.031	12	400	44.58
1.970	<1	410	46.04
1.914	1	330	47.46
1.863	20	331	48.85
1.816	17	420	50.19
1.772	1	421	51.53
1.732	1	332	52.82
1.658	13	422	55.37
1.5923	<1	510	57.86
1.5626	11	333	59.07
1.5079	1	432	61.44
1.4827	<1	521	62.60
1.4352	8	440	64.92
1.3919	1	530	67.20
1.3723	15	531	68.29
1.3532	7	600	69.39
1.3348	1	610	70.49
1.3171	1	611	71.58
1.2836	3	620	73.75
1.2681	<1	621	74.81
1.2380	5	533	76.95
1.2237	5	622	78.02
1.2103	<1	630	79.05
1.1719	2	444	82.19
1.1367	5	551	85.32
1.1259	2	640	86.34
1.1151	1	720	87.38
1.0848	4	642	90.48
1.0570	5	731	93.56
1.0149	<1	800	98.75
1.0071	<1	740	99.79
.9918	1	733	101.91
.9844	2	820	102.98
.9567	2	660	107.24
.9375	3	751	110.50
.9313	1	662	111.61
.9078	1	840	116.11
.8910	2	911	119.65
.8857	1	842	120.84
.8654	1	664	125.76
.8510	1	931	129.69
.8285	1	844	136.80
.8158	2	755	141.53
.8119	1	860	143.17
.7960	2	10·2·0	150.78
.7848	<1	951	157.94

References

Birnstock, R. (1967). Z. Krist. 124, 310.
Swanson, H.E. and Tatge,E. (1953). Natl. Bur. Std. U.S. Circ. 539, 1, 81.

Cadmium bromide chloride, CdBrCl

Sample

The sample was prepared by melting a 1:1 molar mixture of $CdBr_2$ and $CdCl_2$. This was then annealed for three days at 300°C in a sealed tube.

Color

Light grey

Structure

Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with $CdCl_2$. The structure of $CdCl_2$ was determined by Pauling [1929]. A complete solid solution exists between $CdBr_2$ and $CdCl_2$ [Nacken, 1907].

NBS lattice constants:

a = 3.9204(3)Å

c =18.408(2)

Density

(calculated) 4.630 g/cm^3

Reference intensity

$I/I_{corundum}$ 3.3

References

Nacken, R. (1907). Centr. Mineral Geol. 1907, 303.

Pauling, L. (1929). Proc. Nat. Acad. Sci. U.S. 15, 709.

Internal standard W, a = 3.16516 Å

$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ (°)
6.137	100	003	14.42
3.340	30	101	26.67
3.068	1	006	29.08
2.734	60	104	32.73
2.496	10	015	35.95
2.081	6	107	43.46
2.046	3	009	44.23
1.961	25	110	46.26
1.905	17	018	47.70
1.868	10	113	48.71
1.690	3	021	54.22
1.5928	7	024	57.84
1.5417	1	205	59.95
1.5338	4	0.0.12	60.29
1.5013	1	0.1.11	61.74
1.4268	1	027	65.35
1.4154	2	119	65.94
1.3662	3	208	68.64
1.3070	<1	1.0.13	72.22
1.2801	2	211	73.99
1.2359	4	214	77.11
1.2272	1	0.0.15	77.76
1.2116	1	125	78.95
1.2079	4	1.1.12	79.24
1.1917	<1	2.0.11	80.53
1.1534	1	217	83.80
1.1317	2	300	85.79
1.1206	2	128	86.85
1.1129	<1	303	87.60
1.0897	1	1.0.16	89.96
1.0400	<1	1.1.15	95.57
1.0315	<1	0.1.17	96.62
1.0183	<1	1.2.11	98.30

Calcium aluminum hydroxide, $Ca_3Al_2(OH)_{12}$

Sample

The sample was prepared by treating a saturated solution of CaO with 6 % phenol. Aluminum metal dissolved in KOH was added. The compound was then dried at 110 °C for two hours.

Color

Colorless

Optical data

Isotropic, N = 1.605

Structure

Cubic, Ia3d (230), Z = 8, garnet type [Flint et al., 1941].

NBS lattice constant:
a = 12.5727(2)Å

Density

(calculated) 2.527 g/cm^3

Reference intensity

$I/I_{corundum} = 1.0$

Additional patterns

1. PDF 3-125 [Flint et al., 1941]

References

Flint, E.P., McMurdie, H.F., and Wells, L.S.(1941) J. Res. Natl. Bur. Std. 26, 13.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.130	90	211	17.27
4.442	40	220	19.97
3.358	55	321	26.52
3.142	45	400	28.38
2.810	80	420	31.82
2.680	6	332	33.41
2.566	15	422	34.94
2.465	30	431	36.42
2.295	100	521	39.23
2.222	4	440	40.56
2.039	95	611	44.39
1.989	8	620	45.58
1.8536	1	631	49.11
1.8148	10	444	50.23
1.7785	2	543	51.33
1.7437	40	640	52.43
1.7111	20	721	53.51
1.6800	50	642	54.58
1.5964	11	732	57.70
1.5715	13	800	58.70
1.5478	1	741	59.69
1.5249	1	820	60.68
1.5030	2	653	61.66
1.4818	3	660	62.64
1.4616	1	831	63.61
1.4243	1	752	65.48
1.4058	12	840	66.45
1.3716	5	842	68.33
1.3555	5	761	69.26
1.3401	8	664	70.17
1.3253	2	851	71.07
1.2965	5	932	72.90
1.2835	2	844	73.76
1.2701	4	941	74.67
1.2449	2	10·1·1	76.45
1.2330	1	10·2·0	77.32
1.2216	1	943	78.18
1.1986	8	10·3·1	79.98
1.1774	<1	871	81.72
1.1673	8	10·4·0	82.58
1.1574	4	10·3·3	83.45
1.1478	10	10·4·2	84.30
1.1382	1	873	85.18
1.1202	8	11·2·1	86.89
1.1113	4	880	87.76

d (Å)	*I*	*hkl*	2θ(°)
1.0863	4	11·3·2	90.32
1.0624	1	10·6·2	92.94
1.0551	2	965	93.78
1.0478	2	12·0·0	94.64
1.0406	1	11·4·3	95.50
1.0337	2	12·2·0	96.35
1.0266	2	11·5·2	97.24
1.0197	5	12·2·2	98.12
1.0132	1	12·3·1	98.97
0.9758	5	11·6·3	104.26
.9532	2	13·2·1	107.83
.9477	1	12·4·4	108.74
.9371	5	12·6·0	110.56
.9320	3	13·3·2	111.47
.9268	3	12·6·2	112.43
.9220	1	13·4·1	113.33
.9073	1	888	116.19
.8935	1	13·5·2	119.11
.8890	1	14·2·0	120.09
.8846	1	12·7·3	121.10
.8760	3	14·3·1	123.13
.8718	2	12·8·0	124.15
.8675	<1	13·5·4	125.23
.8635	3	14·4·0	126.26
.8593	<1	14·3·3	127.38
.8554	8	14·4·2	128.44

Calcium chloride (hydrophilite), $CaCl_2$

Sample

$CaCO_3$ was slowly converted to $CaCl_2$ by exposure to dry HCl fumes. However, since a few peaks of another phase persisted in the sample it was felt that intensity values should be calculated rather than measured.

Color

Colorless

Structure

Orthorhombic, Pnnm (58), Z=2, distorted rutile arrangement. The structure was determined by van Bever and Nieuwenkamp [1935]. Intensity values were calculated from structure data using the following information:

NBS lattice constants:
a = 6.261(2)Å
b = 6.429(2)
c = 4.167(1)

Atom positions:
Ca (0 0 0)
Cl (.275 .325 0) [van Bever and Nieuwenkamp, 1935]

Scattering factors:
Ca^{2+}, Cl^- [International Tables, 1962]

Thermal parameters:
overall B = 1.0

Density

(calculated) 2.175 g/cm³

Polymorphism

Jensen [1943] described 3 modifications.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I* (calc.)	*hkl*	2θ(°)
4.48	85	110	19.80
3.46	17	101	25.71
3.050	100	111	29.26
2.858	35	120	31.27
2.816	4	210	31.75
2.356	25	121	38.16
2.331	50	211	38.59
2.244	30	220	40.16
2.083	20	002	43.40
2.027	3	130	44.66
1.974	2	221	45.94
1.906	25	031	47.68
1.890	10	112	48.10
1.866	11	301	48.75
1.792	10	311	50.92
1.751	4	320	52.20
1.684	7	122	54.44
1.565	4	400	58.97
1.527	10	222	60.59
1.496	4	330	62.00

Additional patterns

1. PDF card 1-0338 [Hanawalt et al., 1938]
2. Döll and Klemm [1939]

References

van Bever, A. K. and Nieuwenkamp, W. (1935). Z. Krist. 90, 374.

Döll, W. and Klemm, W. (1939). Z. anorg. u. allgem. Chem. 241, 233.

Hanawalt, J.D., Rinn, H.W., and Frevel, L.K.(1938) Ind. Eng. Chem. Anal. Ed. 10, 457.

International Tables III (1962). 202, 204.

Jensen, A.T. (1943). Kgl. Danske Videnskab. Selskab 20 #5, 1.

Cesium cobalt chloride, Cs_2CoCl_4

Sample
The sample was prepared by slow evaporation at room temperature of a 2:1 aqueous solution of CsCl and $CoCl_2$.

Color
Brilliant greenish blue

Optical data
Biaxial, $N_\alpha = 1.575$, $N_\beta = 1.585$, $N_\gamma = 1.596$; 2V is very large.

Structure
Orthorhombic, Pnam (62), Z=4, isostructural with K_2SO_4 and Cs_2CuCl_4 [Porai-Koshitz, 1954]. The structure was determined by Tishchenko and Pinsker [1955].

NBS lattice constants:
a = 9.771(2)Å
b = 12.973(2)
c = 7.401(1)

Density
(calculated) 3.303 g/cm³

Reference intensity
$I/I_{corundum}$ 1.8

Major impurities
~ .05% Al, Cu, Si, and Zn.

References

Porai-Koshitz, M.A. (1954). Tr. Inst. Kristallogr. Akad. Nauk SSSR **10**, 269.
Tishchenko, G.N. and Pinsker, Z.G. (1955). Dokl. Akad. Nauk SSSR **100**, 913.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.569	18	210	19.41
4.367	90	121	20.32
4.075	15	201	21.79
3.952	19	130	22.48
3.889	75	211	22.85
3.731	95	031	23.83
3.697	100	002	24.05
3.485	10	131	25.54
3.454	10	221	25.77
3.345	4	112	26.63
3.242	70	040	27.49
3.157	75	310	28.24
3.075	14	140	29.01
3.053	35	122	29.23
2.947	11	202	30.30
2.904	40	311	30.76
2.875	55	212	31.08
2.841	30	141	31.46
2.700	35	240,132	33.15
2.684	30	222	33.36
2.600	40	330	34.46
2.537	8	241	35.35
2.507	12	150	35.78
2.447	20	051	36.70
2.436	40	232	36.87
2.402	20	312,410	37.41
2.319	5	401	38.80
2.297	8	340	39.18
2.284	16	411	39.42
2.245	13	123	40.14
2.194	19	341	41.11
2.170	10	213	41.59
2.142	13	033	42.16
2.126	9	332,430	42.48
2.093	2	133	43.18
2.086	4	223	43.35
2.076	11	152	43.57
1.976	6	260	45.88
1.951	11	342,440	46.50
1.945	13	422,313	46.66
1.925	6	143	47.17
1.910	5	261	47.56
1.870	13	520,511	48.65
1.850	16	004	49.21
1.843	13	432	49.40
1.822	3	243,170	50.03
1.798	10	071	50.74
1.779	5	352,024 +	51.30
1.750	5	124,361	52.24
1.744	14	262	52.41
1.730	6	531,204	52.88
1.714	7	512	53.42
1.687	3	271	54.32
1.682	8	343	54.50
1.670	18	522	54.93
1.632	9	541	56.31
1.629	8	600	56.45
1.622	3	080	56.69
1.6068	11	044	57.29
1.6037	9	163,452	57.41
1.6004	10	180	57.54
1.5969	9	314	57.68
1.5911	7	601	57.91
1.5858	4	144	58.12
1.5431	2	263	59.89
1.5276	7	551	60.56
1.5081	6	334	61.43
1.4891	5	154	62.30

Sample

The sample was prepared by slow evaporation at room temperature of a 2:1 molar aqueous solution of CsCl and $CuCl_2$.

Color

Unground - deep brown
Ground - deep orange

Optical data

Biaxial (+), $N_\alpha = 1.625$, $N_\beta = 1.648$, $N_\gamma = 1.678$
2V = 83° 46' [Helmholz and Kruh, 1952].

Structure

Orthorhombic, Pnam (62), Z = 4. The space group was determined by Mellor [1939]. The structure was determined by Helmholz and Kruh [1952], and refined by Morosin and Lingafelter [1961].

NBS lattice constants:
a = 9.773(2)Å
b = 12.415(2)
c = 7.617(2)

Density

(calculated) 3.386 g/cm^3

Reference intensity

$I/I_{corundum} = 1.2$

References

Helmholz, L. and Kruh, R.F. (1952). J. Am. Chem. Soc. 74, 1176.
Mellor, D.P. (1939). Z. Krist. 101A, 160.
Morosin, B. and Lingafelter, E.C. (1961). J. Phys. Chem. 65, 50.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.236	2	120	16.92
4.546	11	210	19.51
4.316	55	121	20.56
4.116	25	201	21.57
3.905	40	211	22.75
3.841	35	220	23.14
3.808	100	130,002	23.34
3.638	50	031	24.45
3.410	5	112,131	26.11
3.247	2	022	27.45
3.157	60	230	28.24
3.152	60	310	28.29
3.103	60	040	28.75
3.082	30	122	28.95
3.005	16	202	29.71
2.959	4	140	30.18
2.920	25	212,231	30.59
2.913	25	311	30.67
2.884	25	320	30.98
2.758	16	141	32.43
2.704	25	222	33.10
2.696	25	321,132	33.20
2.560	30	330	35.02
2.477	12	241	36.23
2.442	9	400	36.77
2.429	35	232,312	36.97
2.406	25	150,042	37.35
2.361	3	051	38.09
2.300	7	322	39.14
2.286	20	411,123	39.38
2.274	6	420	39.60
2.253	5	203	39.99
2.247	3	340	40.09
2.217	12	213	40.67
2.179	2	421	41.40
2.164	11	033	41.71
2.156	13	242,341	41.87
2.124	10	251,332	42.53
2.056	2	402	44.00
2.033	11	152	44.52
2.028	10	412,431	44.64
1.980	5	233	45.79
1.977	3	313,350	45.86
1.953	3	422	46.47
1.935	5	342	46.92
1.929	7	510,143	47.06
1.910	8	351	47.56
1.904	25	260,004	47.72
1.872	5	511	48.60
1.864	7	520	48.82

d (Å)	I	hkl	2θ(°)
1.848	2	261,114	49.26
1.842	4	432	49.45
1.823	3	243	49.99
1.819	4	062	50.12
1.788	4	124,162	51.04
1.7673	3	530	51.68
1.7562	2	214	52.03
1.7428	5	413	52.46
1.7269	14	071	52.98
1.7218	16	512,531	53.15
1.7031	17	262,134	53.78
1.6979	11	451	53.96
1.6826	4	343	54.49
1.6746	6	522	54.77
1.6668	4	270	55.05
1.6546	3	540	55.49
1.6298	12	314,600	56.41
1.6234	8	044	56.65
1.6169	9	541	56.90
1.6030	9	532	57.44
1.5886	6	324	58.01
1.5786	6	611,460	58.41
1.5590	3	353	59.22
1.5366	3	513,550	60.17
1.5276	9	334,272	60.56
1.5166	5	542	61.05

Cobalt chloride hydrate, $CoCl_2 \cdot 2H_2O$

Sample

The sample was prepared by evaporating an aqueous solution of $CoCl_2$ at about 90 °C. The first crystals formed were filtered from the solution and washed with ethyl alcohol. The sample forms a higher hydrate in moist air.

Color

Deep violet

Structure

Monoclinic, C2/m (12), Z = 2, isostructural with $CoBr_2 \cdot 2H_2O$ and the corresponding Mn salts [Morosin, 1965]. The structure of $CoBr_2 \cdot 2H_2O$ was determined by Morosin and Graeber [1963].

NBS lattice constants:

a = 7.280(1)Å
b = 8.552(2)
c = 3.573(1)
β = 97.55(1)°

Density

(calculated) 2.498 g/cm^3

Reference intensity

$I/I_{corundum} = 2.5$

Additional patterns

1. PDF card 3-786 [Neuhaus, 1938].

References

Morosin, B. (1965). Abstract Bull. Am. Phys. Soc. 10, 686.

Morosin, B. and Graeber, E.J. (1963). Acta Cryst. 16, 1176.

Neuhaus, A. (1938). Z. Krist. 98, 112.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.514	100	110	16.06
4.277	65	020	20.75
3.606	2	200	24.67
3.542	3	001	25.13
3.127	4	$\bar{1}11$	28.52
2.854	25	111	31.32
2.758	14	220	32.43
2.726	20	021	32.83
2.712	40	$\bar{2}01$	33.00
2.651	11	130	33.78
2.376	25	201	37.84
2.315	4	$\bar{3}10$	38.87
2.291	12	$\bar{2}21$	39.30
2.138	20	040	42.23
2.076	19	131,221	43.56
2.0611	12	$\bar{3}11$	43.89
1.8350	4	311	49.64
1.8044	8	400	50.54
1.7711	6	002	51.56
1.7379	6	$\bar{1}12$	52.62
1.7031	5	$\bar{3}31$	53.78
1.6789	10	$\bar{2}41$	54.62
1.6626	6	420	55.20
1.6359	3	022	56.18
1.5896	10	241	57.97
1.4233	3	510	65.53
1.3938	1	350	67.09
1.3786	5	440	67.94

Cobalt chloride hydrate, $CoCl_2 \cdot 6H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of an aqueous solution of $CoCl_2$.

Color
Deep purplish red

Optical data
Biaxial (+), N_α=1.524, N_β=1.548, N_γ=1.580. 2V is very large.

Structure
Monoclinic, I2/m (12), Z = 2, isostructural with $NiCl_2 \cdot 6H_2O$. The structure was determined by Mizuno (1960).

NBS lattice constants:
a = 8.898(2)Å
b = 7.066(1)
c = 6.644(1)
β = 97.25(1)°

Density
(calculated) 1.907 g/cm^3

Polymorphism
1. PDF card 13-399 [Inst. of Physics, University College, Cardiff, Wales] reports a cell related to this form but with the c doubled and with space group $P2_1/c$ (14). The pattern however appears quite different, so a polymorph may exist.

References
Mizuno, J. (1960). J. Phys. Soc. Japan **15**, 1412.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.636	100	$\bar{1}01$	15.71
5.521	45	110	16.04
4.987	15	101	17.77
4.826	55	011	18.37
4.421	4	200	20.07
3.534	18	020	25.18
3.414	4	$\bar{2}11$	26.08
3.115	11	211	28.63
2.993	16	$\bar{1}21$	29.83
2.933	55	$\bar{1}12$	30.45
2.817	20	$\bar{2}02$	31.74
2.758	30	220	32.44
2.735	16	112	32.72
2.716	35	310	32.95
2.569	19	301	34.89
2.410	30	022	37.28
2.219	10	031	40.63
2.206	25	400,$\bar{3}21$	40.87
2.079	10	$\bar{4}11$,321	43.49
2.038	7	222	44.41
1.985	18	$\bar{3}12$	45.66
1.951	5	$\bar{4}02$,231	46.51
1.940	5	411	46.80
1.902	17	$\bar{1}32$	47.77
1.871	8	420	48.62
1.8664	8	$\bar{1}23$	48.75
1.8388	4	330	49.53
1.8118	4	213	50.32
1.7873	3	123	51.06
1.7666	7	040	51.70
1.7075	15	$\bar{4}22$	53.63
1.6852	3	$\bar{1}41$	54.40
1.6136	9	$\bar{1}14$	57.03
1.6115	8	$\bar{2}04$	57.11
1.5989	6	$\bar{4}31$	57.60
1.5769	3	$\bar{5}21$	58.48
1.5564	10	042,$\bar{2}33$	59.33
1.5540	6	332	59.43
1.5041	4	323	61.61
1.4932	3	024	62.11
1.4837	3	204	62.55
1.4694	5	$\bar{5}03$	63.23
1.4665	5	233,$\bar{2}24$	63.37
1.4554	3	341	63.91

Cobalt fluoride hydrate, $CoF_2 \cdot 4H_2O$

Sample

The sample was prepared by slow evaporation of an aqueous solution of CoF_2 at room temperature.

Color

Medium red

Structure

Orthorhombic, $P2_1ab$ (29), Z = 4, isostructural with $ZnF_2 \cdot 4H_2O$ and other similar tetrahydrates. The structure of $ZnF_2 \cdot 4H_2O$ was investigated by Rao et al. [1965].

NBS lattice constants:

a = 7.552(2)Å
b = 12.658(3)
c = 5.287(1)

Density

(calculated) 2.221 g/cm^3

Reference intensity

$I/I_{corundum}$ = 1.8

Polymorphism

Easwaran and Srinivasan [1965] reported, by comparison of powder patterns, that $CoF_2 \cdot 4H_2O$ was isostructural with $FeF_2 \cdot 4H_2O$. However, Penfold and Taylor [1960] reported $FeF_2 \cdot 4H_2O$ as rhombohedral. This suggests a second form of $CoF_2 \cdot 4H_2O$ exists.

Additional patterns

1. PDF card 1-258 [Hanawalt et al., 1938]

References

Easwaran, K.R.K. and Srinivasan, R. (1965). Proc. Nuclear Physics - Solid State Physics Symposium, Calcutta, Part A, 171.

Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. **10**, 457.

Penfold, B.R. and Taylor, M.R. (1960). Acta Cryst. **13**, 953.

Rao, K.V.K., Naidu, S.V.N., and Rao, P.V. (1965). Indian J. Pure Applied Phys. **3**, 68.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.289	5	001	16.75
4.854	100	120, 011	18.26
4.096	35	111	21.68
3.776	4	200	23.54
3.577	3	121	24.87
3.296	4	031	27.03
3.165	25	040	28.17
3.071	3	201	29.05
3.019	5	131	29.56
2.987	30	211	29.89
2.919	2	140	30.60
2.764	15	221	32.36
2.644	1	002	33.88
2.589	3	012	34.62
2.557	7	141	35.07
2.484	3	231	36.13
2.448	5	112	36.68
2.338	3	320	38.48
2.321	4	122	38.76
2.281	2	051	39.47
2.237	7	311	40.29
2.186	8	151	41.26
2.165	14	202	41.68
2.136	4	212	42.28
2.031	20	160	44.58
2.001	4	331	45.28
1.959	6	061,142	46.31
1.954	7	251	46.44
1.927	3	232	47.12
1.889	6	400	48.14
1.845	1	341	49.34
1.8044	5	312	50.54
1.7869	8	242	51.07
1.7606	5	411	51.89
1.7515	11	322	52.18
1.7465	7	013	52.34
1.7117	2	421,071	53.49
1.6921	2	351	54.16
1.6732	3	332	54.82
1.6696	3	171	54.95
1.6563	3	123	55.43
1.6456	3	252	55.82
1.6213	3	440	56.73
1.6169	3	360	56.90
1.5893	2	133	57.98

Copper fluoride hydrate, $CuF_2 \cdot 2H_2O$

Sample
The sample was prepared by slow evaporation of a CuF_2 aqueous solution at room temperature.

Color
Brilliant greenish blue

Optical data
Biaxial (-), N_α=1.502, N_β=1.522, N_γ=1.534; 2V is medium large.

Structure
Monoclinic, I2/m (12), Z=2. The structure was determined by Abrahams and Prince [1962] using neutron diffraction.

NBS lattice constants:
a = 6.412(1)Å
b = 7.403(1)
c = 3.3025(6)
β = 99.46(1)°

Density
(calculated) 2.954 g/cm^3

Reference intensity
$I/I_{corundum}$ 2.5

Additional patterns
1. PDF card 6-143 [Wheeler and Haendler, 1954].

References

Abrahams, S. C. and Prince, E. (1962). J. Chem. Phys. 36, 50.
Wheeler, C.M.Jr. and Haendler, H.M. (1954). J. Am. Chem. Soc. 76, 263.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.805	100	110	18.45
3.700	30	020	24.03
3.164	17	$\bar{2}00$	28.18
3.113	15	$\bar{1}01$	28.65
2.983	12	011	29.93
2.717	45	101	32.94
2.404	<1	$\bar{2}20$	37.37
2.353	15	$\bar{2}11$	38.22
2.299	20	130	39.16
2.191	8	121	41.16
2.023	15	211	44.77
1.968	6	031	46.08
1.919	13	$\bar{3}01$	47.32
1.850	11	040	49.20
1.750	6	$\bar{2}31$	52.24
1.704	5	$\bar{3}21$	53.75
1.650	2	301	55.64
1.629	<1	002	56.44
1.601	12	231	57.51
1.5818	5	400	58.28
1.5556	4	$\bar{2}02$	59.36
1.5299	6	141	60.46
1.5079	<1	321	61.44
1.4930	2	$\bar{4}11$	62.12
1.4906	<1	022	62.23
1.4544	<1	420	63.96
1.4413	<1	150	64.61
1.4342	<1	$\bar{2}22$	64.97
1.3685	1	$\bar{1}32$	68.51
1.3598	<1	202	69.01
1.3325	4	$\bar{3}41$	70.63

Sample

The sample was made by I. Mayer [Hebrew University, Jerusalem]. A mixture of $(NH_4)_2HPO_4$ and Eu_2O_3 was heated at 500 °C for 2 hours, then at 1100 °C overnight.

Color

Colorless

Structure

Monoclinic, $P2_1/n$ (14), Z=4, isostructural with monazite [Feigelson, 1964]. The structure of monazite was determined by Kokkoros [1942].

NBS lattice constants:
a = 6.6684(5)Å
b = 6.8671(5)
c = 6.3534(5)
β = 103.94(1)°

Density

(calculated) 5.808 g/cm³

Additional patterns

1. PDF card 18-506 [Bril and Wanmaker, 1964]

References

Bril, A. and Wanmaker, W.L.(1964). J. Electrochem. Soc. **111**, 1363.
Kokkoros, P. (1942). Prakt. Akad. Anthenon **17**, 163.
Feigelson, R.S. (1964). J. Am. Ceram. Soc. **47**, 257.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.127	12	$\bar{1}01$	17.28
4.714	9	110	18.81
4.593	25	011	19.31
4.107	40	$\bar{1}11$	21.62
4.008	18	101	22.16
3.461	17	111	25.72
3.435	15	020	25.92
3.237	55	200	27.53
3.084	7	002	28.93
3.034	100	120	29.41
3.000	5	021	29.76
2.928	15	$\bar{2}10$	30.51
2.901	6	$\bar{2}11$	30.80
2.813	85	$\bar{1}12$,012	31.79
2.561	25	$\bar{2}02$	35.01
2.446	2	$\bar{2}11$	36.71
2.399	18	$\bar{2}12$	37.45
2.395	19	112	37.52
2.355	6	$\bar{2}20$	38.18
2.342	1	$\bar{2}21$	38.41
2.296	5	$\bar{1}22$,022	39.21
2.208	3	$\bar{3}01$	40.83
2.146	25	031	42.07
2.112	25	$\bar{1}03$	42.79
2.104	25	$\bar{3}11$	42.96
2.081	19	221	43.44
2.058	2	$\bar{3}10$	43.96
2.053	3	$\bar{2}22$	44.08
1.988	2	131	45.60
1.923	35	212	47.22
1.899	6	301	47.87
1.868	3	$\bar{2}30$	48.70
1.862	14	$\bar{2}31$	48.88
1.839	25	$\bar{1}32$,032	49.53
1.835	15	103	49.64
1.827	15	$\bar{3}20$	49.87
1.7988	2	$\bar{1}23$	50.71
1.7737	2	113	51.48
1.7638	11	023	51.79
1.7339	19	$\bar{3}22$	52.75
1.7227	4	231	53.12
1.7170	5	040	53.31
1.7043	25	132,$\bar{2}23$	53.74
1.6593	11	$\bar{1}40$	55.32
1.6377	1	$\bar{1}41$	56.49
1.6180	4	123,$\bar{4}00$	56.86
1.6002	7	$\bar{4}02$	57.55
1.5782	2	141	58.43
1.5750	7	410	58.56
1.5701	7	330	58.76

d (Å)	I	hkl	2θ(°)
1.5583	2	$\bar{4}12$	59.25
1.5547	4	312	59.40
1.5476	2	$\bar{1}14$	59.70
1.5420	5	004	59.94
1.5322	2	213	60.36
1.5288	1	033,$\bar{3}$23	60.51
1.5168	3	240	61.04
1.5101	5	$\bar{3}$32	61.34
1.5059	10	$\bar{2}$14	61.53
1.5003	4	$\bar{1}$42,042	61.78
1.4503	2	$\bar{4}$22	64.16
1.4473	1	322,411	64.31
1.4417	4	$\bar{1}$24	64.59
1.4358	3	241	64.89
1.4322	2	133	65.07
1.4295	3	223	65.21
1.4260	3	$\bar{2}$42	65.39
1.4062	1	024	66.43
1.3974	3	$\bar{3}$14	66.90
1.3591	2	421	69.05
1.3473	4	$\bar{4}$31	69.74
1.3434	5	150,340	69.97
1.3379	3	$\bar{4}$23	70.30
1.3320	3	$\bar{1}$43	70.66
1.3263	2	$\bar{1}$51	71.01
1.3179	4	$\bar{3}$24,043	71.53
1.3152	7	124	71.70
1.3091	11	332,402	72.09
1.3052	10	$\bar{3}$42,$\bar{1}$34	72.34

Glucose, D, alpha, (dextrose), $C_6H_{12}O_6$

Sample

The sample was NBS Standard Reference Material 41a. The dextrose was produced by Pfanstiehl Laboratories, Inc. Chicago, Illinois

moisture.....	less than 0.02%
ash.....	less than 0.01%

Color

Colorless

Structure

Orthorhombic, $P2_12_12_1(19)$. Z=4, [Sponsler and Dove, 1931]. The structure was determined by McDonald and Beevers [1952].

NBS lattice constants:

a = 10.368(2)Å
b = 14.856(2)
c = 4.9808(6)

Density

(calculated) 1.560 g/cm^3

Reference intensity

$I/I_{corundum} = 2.3$

Additional patterns

1. PDF card 1-374 [Sponsler and Dove, 1931]
2. PDF card 3-228 Inst. of Physics at University College, Cardiff, Wales.

References

McDonald, T.R.R. and Beevers, C.A. (1952). Acta Cryst. **5**, 654.

Sponsler, O.L. and Dove, W.H. (1931). J. Am. Chem. Soc. **53**, 1639.

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
8.50	7	110	10.40
7.42	6	020	11.91
6.04	15	120	14.66
5.181	14	200	17.10
4.894	1	210	18.11
4.724	20	011	18.77
4.487	4	101	19.77
4.298	100	111	20.65
4.251	8	220	20.88
3.841	4	121	23.14
3.709	1	040	23.97
3.590	4	201	24.78
3.493	11	140,211	25.48
3.366	2	310	26.46
3.326	3	131	26.78
3.234	2	221	27.56
3.132	19	320	28.47
3.018	1	240	29.57
2.977	2	041	29.99
2.907	4	231	30.73
2.856	4	150	31.29
2.833	1	330	31.55
2.789	<1	311	32.06
2.651	2	321	33.78
2.590	5	400	34.60
2.581	4	241	34.73
2.551	4	410,051	35.15
2.530	2	340	35.45
2.489	8	002	36.05
2.477	9	151,060	36.23
2.455	7	012	36.57
2.449	7	420	36.67
2.423	2	102	37.08
2.408	1	160	37.31
2.390	1	112	37.60
2.362	7	022	38.07
2.295	4	430	39.22
2.273	4	411	39.62
2.255	6	341	39.94
2.233	1	260	40.35
2.217	4	061	40.66
2.196	1	421	41.06
2.168	1	161	41.62
2.150	1	222	41.99
2.125	<1	440	42.51
2.085	1	431	43.36
2.080	1	170	43.47
2.053	4	510,351	44.08
2.002	1	312	45.26
1.963	2	270	46.20

d (Å)	*I*	*hkl*	2θ(°)
1.953	2	450,071	46.47
1.918	2	171	47.36
1.914	2	501,530	47.47
1.899	1	511	47.87
1.867	1	361	48.74
1.854	1	521	49.10
1.827	1	180,271	49.87
1.818	<1	451	50.14
1.809	<1	370	50.40
1.791	2	252,460	50.95
1.786	1	531	51.10
1.775	<1	342	51.43
1.756	1	062	52.05
1.745	<1	422	52.39
1.741	<1	081	52.52
1.716	<1	610,181	53.35
1.701	1	541,550+	53.86
1.684	1	461,620	54.44
1.671	1	352	54.90
1.663	1	262	55.18
1.650	<1	013,281	55.66
1.630	1	190,113	56.39
1.623	1	611	56.65
1.617	<1	442	56.90
1.601	1	123	57.53
1.595	2	172,621	57.75
1.5811	1	203	58.31
1.5664	1	091,640+	58.91

Sample

The In_2S_3 was made by W.S. Brower by heating the elements in a sealed silica tube at 460 °C for sixteen hours and at 880 °C for six hours.

Color

Unground: dark grayish red

Ground: strong reddish brown

Structure

Tetragonal, $I4_122$ (98), Z=16. The structure was studied by Rooymans [1959] and by Goodyear and Steigmann [1961].

NBS lattice constants:
a = 7.619(1)Å
c = 32.329(4)

Density

(calculated) 4.613 g/cm³

Reference intensity

$I/I_{corundum} = 4.2$

Polymorphism

Hahn and Klinger [1949] found that a low temperature form transformed irreversibly at about 330 °C to a high form which they indexed as cubic with a few extra non-cubic lines.

Additional patterns

1. Goodyear and Steigmann [1961].

References

Goodyear, J. and Steigmann, G.A. (1961). Proc. Phys. Soc. **78** 491.

Hahn, H. and Klinger, W. (1949). Z. anorg. Chem. **260**, 97.

Rooymans, C.J.M. (1959). J. Inorg. Nucl. Chem. **11**, 78.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
8.09	4	004	10.93
7.40	3	101	11.95
6.21	30	103	14.24
5.110	12	112	17.34
4.927	2	105	17.99
4.041	3	008	21.98
3.947	2	107	22.51
3.811	18	200,116	23.32
3.445	2	204	25.84
3.392	2	211	26.25
3.249	100	109,213	27.43
3.112	12	206	28.66
3.015	1	215	29.60
2.770	3	208,1·1·10	32.29
2.741	3	1·0·11,217	32.64
2.694	50	0·0·12,220	33.23
2.557	1	224	35.07
2.532	1	301	35.42
2.472	4	219,303	36.31
2.382	1	312	37.74
2.364	3	1·0·13,305	38.04
2.309	1	314	38.97
2.225	3	2·1·11,307	40.51
2.199	9	2·0·12,316	41.00
2.123	1	1·1·14	42.54
2.107	2	321	42.88
2.074	45	309,323	43.61
2.009	3	2·1·13,325	45.09
1.905	65	2·2·12,400	47.71
1.845	1	1·0·17,411	49.34
1.8213	6	329,413,+	50.04
1.7766	1	3·0·13,415	51.39
1.7224	1	334,408,+	53.13
1.7161	1	3·2·11,417	53.34
1.7037	3	336,420,+	53.76
1.6673	3	3·1·14,424	55.03
1.6615	3	1·0·19,2·1·17	55.24
1.6429	13	3·0·15,419	55.92
1.6242	5	426,2·0·18	56.62
1.6161	3	2·2·16,0·0·20	56.93
1.5701	2	3·3·10,428	58.76
1.5647	2	4·1·11	58.98
1.5556	10	4·0·12	59.36
1.5224	1	2·1·19,431,+	60.79
1.5090	4	1·0·21,3·2·15	61.39
1.4876	3	2·0·20,512	62.37
1.4835	2	4·1·13,435	62.56
1.4475	1	437	64.30
1.4403	4	3·1·18,516,+	64.66
1.4181	2	1·1·22,3·3·14	65.80

d (Å)	I	hkl	2θ(°)
1.4137	2	3·0·19,521,+	66.03
1.4028	16	439,523,+	66.61
1.3527	2	4·3·11,527	69.42
1.3470	8	440,0·0·24	69.76
1.3252	1	3·2·19,4·1·17	71.08
1.2746	1	1·0·25,5·2·11	74.36
1.2701	2	2·0·24,536,+	74.67
1.2442	9	4·3·15,613,+	76.50
1.2364	2	4·2·18,606	77.07
1.2301	2	3·0·23,615,+	77.54
1.2119	1	1·1·26,608,+	78.93
1.2046	6	4·4·12,620,+	79.49
1.1895	1	4·3·17,541	80.72
1.1829	1	1·0·27,619,+	81.26
1.1728	1	4·2·20	82.11
1.1524	1	3·0·25,547,+	83.89
1.1488	1	5·1·18,6·0·12	84.21
1.1294	5	549,633,+	86.00
1.1190	1	4·1·23,635,+	87.00
1.0997	14	4·0·24,6·2·12	88.93
1.0832	<1	3·0·27,639,+	90.65
1.0566	2	556,640,+	93.61
1.0462	2	6·1·17,721	94.83
1.0418	7	3·2·27,709,+	95.36
1.0368	4	6·0·18,646,+	95.97
1.0334	3	1·0·31,725,+	96.38
1.0223	1	5·5·10,648,+	97.79
1.0048	1	6·3·15,729	100.10
0.9715	2	7·0·15,653,+	104.91
.9524	4	4·4·24,800	107.96
.9413	1	659,743,+	109.83

Sample

The sample was prepared by permitting anhydrous $FeCl_2$ to hydrate in humid air. The sample was somewhat hygroscopic.

Color

light yellowish brown

Structure

Monoclinic, C2/m (12), Z=2, isostructural with $CoCl_2 \cdot 2H_2O$ and $MnCl_2 \cdot 2H_2O$. The structure was determined by Morosin and Graeber [1965].

NBS lattice constants:

a = 7.3523(6)Å
b = 8.5609(8)
c = 3.6367(3)
β = 98.10(1)°

Density (calculated) 2.385 g/cm³

Additional patterns

1. PDF card 1-210 [Hanawalt et al., 1938]

References

Hanawalt, J.D., Rinn, H.W.,and Frevel, L.K.(1938). Ind. Eng. Chem. Anal. Ed. **10**, 457.

Morosin, B. and Graeber, E. J. (1965). J. Chem. Phys. **42**, 898.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.548	100	110	15.96
4.281	75	020	20.73
3.641	7	200	24.43
3.600	7	001	24.71
3.181	8	$\bar{1}11$	28.03
2.884	45	111	30.98
2.773	45	220	32.25
2.763	90	$\bar{2}01$	32.38
2.657	25	130	33.70
2.396	45	201	37.50
2.335	12	310	38.53
2.321	25	$\bar{2}21$	38.77
2.193	5	$\bar{1}31$	41.13
2.141	35	040	42.18
2.092	45	$\bar{3}11,221$	43.21
2.088	35	131	43.30
1.848	7	330,311	49.26
1.840	6	041	49.51
1.820	19	400	50.09
1.800	13	002	50.67
1.769	14	$\bar{1}12$	51.62
1.721	9	$\bar{3}31$	53.18
1.711	7	$\bar{2}02$	53.49
1.692	20	$\bar{2}41$	54.17
1.674	11	420	54.79
1.6668	9	150	55.05
1.6609	8	112	55.26
1.6593	7	022	55.32
1.5959	18	241	57.72
1.5772	4	331	58.47
1.5313	4	$\bar{1}51$	60.40
1.5270	7	$\bar{1}32$	60.59
1.4943	6	151	62.06
1.4485	3	421	64.25
1.4352	4	510	64.92
1.4268	5	060	65.35
1.3987	3	350	66.83
1.3863	9	440	67.51
1.3775	8	$\bar{0}42$	68.00
1.3408	6	$\bar{3}51,312$	70.13
1.3263	<4	$\bar{0}61$	71.01
1.3138	<4	$\bar{4}22$	71.79
1.2966	<4	530	72.89
1.2739	<4	511	74.41
1.2693	<4	351	74.72
1.2677	4	$\bar{2}61$	74.83
1.2432	4	$\bar{1}52$	76.57
1.2254	4	261,332	77.89
1.2065	4	$\bar{5}12,170$	79.35
1.2021	4	$\bar{6}01$	79.70
1.1981	4	402	80.02
1.1906	<4	$\bar{2}03$	80.63
1.1741	<4	$\bar{5}31$	82.00
1.1605	4	$\bar{4}42$	83.17
1.1572	4	$\bar{6}21$	83.46
1.1536	4	422	83.78
1.1481	4	$\bar{1}13$	84.28
1.1472	4	$\bar{2}23$	84.36
1.1357	<4	$\bar{1}71$	85.41
1.1317	<4	$\bar{3}13$	85.78

Sample

The sample was prepared by melting a 1:1 mixture of $PbCl_2$ and $PbBr_2$. The sample was then ground and annealed in a sealed glass tube at 400 °C overnight.

Color

Colorless

Structure

Orthorhombic, Pnam (62), Z=4, isostructural with $BaCl_2$. There is a complete solid solution series between $PbBr_2$ and $PbCl_2$ [Calingaert et al.,1949] The structure of $PbCl_2$ was determined by Bräkken and Harang [1928].

NBS lattice constants:

a = 7.801(1)Å
b = 9.207(1)
c = 4.5803(5)

Density

(calculated) 6.512 g/cm^3

Reference intensity

$I/I_{corundum} = 2.0$

References

Bräkken, H. and Harang, L. (1928). Z. Krist. 68, 123.

Calingaert, G., Lamb, F.W., and Meyers, F. (1949). J. Am. Chem. Soc. 71, 3712.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.949	2	110	14.88
4.607	6	020	19.25
4.101	17	011	21.65
3.964	80	120	22.41
3.897	30	200	22.80
3.632	90	111	24.49
2.998	30	121	29.78
2.976	20	220	30.00
2.856	16	130	31.29
2.826	100	211	31.64
2.550	50	031	35.17
2.503	8	310	35.84
2.496	3	221	35.95
2.423	16	131	37.07
2.302	40	040	39.09
2.291	40	002	39.30
2.264	40	320	39.78
2.207	10	140	40.85
2.196	40	311	41.06
2.134	40	231	42.32
2.051	1	022	44.12
2.030	1	321	44.61
1.982	30	122,240	45.74
1.949	10	400	46.55
1.908	1	410	47.63
1.821	1	331,241	50.05
1.815	5	222	50.22
1.795	1	420,401	50.83
1.7922	3	150	50.91
1.7869	4	132	51.07
1.7616	2	411	51.86
1.7239	1	340	53.08
1.7090	1	051	53.58
1.6895	3	312	54.25
1.6682	16	151	55.00
1.6229	10	042	56.67
1.6102	20	322	57.16
1.5896	3	142	57.97
1.5647	3	251	58.98
1.5488	7	431	59.65
1.5348	2	060	60.25
1.5052	8	013,160	61.56
1.4984	6	332,242	61.87
1.4874	6	440	62.38
1.4846	10	402	62.51
1.4786	9	113	62.79
1.4663	1	412	63.38
1.4581	12	511	63.78
1.4278	16	260,351	65.30
1.4245	4	123	65.47

d (Å)	I	hkl	2θ(°)
1.4111	1	152	66.17
1.4052	8	213	66.48
1.3770	1	342	68.03
1.3672	6	033	68.58
1.3463	2	252,133	69.80
1.3310	4	531	70.72
1.3216	1	360	71.30
1.3030	4	313	72.48
1.2900	5	233	73.33
1.2751	1	062	74.33
1.2639	5	071	75.10
1.2580	3	162	75.51
1.2479	3	171,442	76.23
1.2416	4	522	76.69
1.2395	3	611	76.84
1.2119	6	262	78.93
1.2025	2	271,403	79.67
1.1920	1	413	80.51
1.1626	3	153	82.99
1.1586	2	631	83.34

Magnesium bromide hydrate, $MgBr_2 \cdot 6H_2O$

Sample

The sample was prepared by treating $MgCO_3$ with a slight excess of an aqueous solution of HBr and evaporating at about 80 °C. The first crystals formed were used.

Color

Colorless

Structure

Monoclinic, C2/m (12), Z = 2, isostructural with $MgCl_2 \cdot 6H_2O$. The structure was determined by Andress and Gundermann [1934].

NBS lattice constants:

a = 10.286(1) Å
b = 7.331(1)
c = 6.211(1)
β = 93.34(1)°

Density

(calculated) 2.076 g/cm³

Reference intensity

$I/I_{corundum} = 2.9$

Additional patterns

1. PDF card 1-1045 [Hanawalt et al., 1938].

References

Andress, K.R. and Gundermann, J. (1934). Z. Krist. 87A, 345.

Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938) Ind. Eng. Chem. Anal. Ed. 10, 457.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
6.20	10	001	14.28
5.133	5	$\underline{2}00$	17.26
4.375	2	$\overline{1}11$	20.28
4.225	100	$\underline{1}11$	21.01
4.070	40	$\overline{2}01$	21.82
3.844	2	201	23.12
3.664	35	020	24.27
3.154	10	021	28.27
3.101	40	310,002	28.77
2.982	30	220	29.94
2.835	18	$\overline{3}11$	31.53
2.791	30	$\underline{\ }\overline{1}12$	32.04
2.724	70	$\overline{2}02,\overline{2}21$	32.85
2.717	55	311,112	32.94
2.655	3	221	33.73
2.589	1	202	34.62
2.568	1	400	34.91
2.423	5	$\overline{4}01$	37.08
2.378	6	130	37.80
2.368	7	022	37.97
2.325	14	$\underline{4}01$	38.70
2.254	1	$\overline{3}12$	39.97
2.210	9	$\overline{1}31$	40.79
2.187	1	$\overline{2}22$	41.25
2.136	4	312	42.27
2.114	6	222	42.73
2.067	1	$\underline{0}03$	43.77
2.037	3	$\overline{4}02$	44.44
2.021	3	$\overline{4}21$	44.80
1.989	4	330	45.58
1.973	4	$\overline{1}13$	45.95
1.963	4	$\underline{4}21$	46.20
1.958	4	$\overline{2}03$	46.34
1.933	2	$\underline{1}13$	46.98
1.915	8	$\overline{5}11$	47.43
1.899	12	$\overline{1}32$	47.86
1.879	6	203	48.39
1.875	10	331,132	48.51
1.8543	2	511	49.09
1.8329	4	040	49.70
1.8004	2	$\underline{0}23$	50.66
1.7804	7	$\overline{4}22$	51.27
1.7634	4	$\overline{3}13$	51.80
1.7266	3	$\overline{2}23,\underline{2}40$	52.99
1.7117	3	600,$\overline{5}12$	53.49
1.7034	2	422	53.77
1.6792	3	313	54.61
1.6718	6	223,$\overline{2}41$	54.87
1.6576	2	$\overline{4}03$	55.38
1.6486	2	332	55.71

d (Å)	I	hkl	2θ(°)
1.6261	2	512,601	56.55
1.5720	2	530	58.68
1.5667	2	403	58.90
1.5504	5	620,004	59.58
1.5403	5	531	60.01
1.5213	2	$\bar{2}42$	60.84
1.5128	4	$\bar{1}14$	61.22
1.5085	3	$\bar{2}04$,531	61.41
1.4958	1	242	61.99
1.4861	2	621	62.44
1.4609	2	$\bar{4}41$,204	63.64
1.4581	2	$\bar{3}33$	63.78
1.4391	4	$\bar{4}41$	64.72
1.4280	2	$\bar{5}32$,024	65.29
1.4189	2	$\bar{7}11$	65.76
1.4156	1	$\bar{1}51$	65.93
1.4103	2	151	66.21
1.3906	1	513	67.27
1.3776	<1	532	67.99
1.3625	2	$\bar{4}04$,$\bar{4}42$	68.85
1.3573	3	$\bar{6}03$,224	69.15
1.3475	2	350	69.73
1.3381	1	$\bar{2}43$	70.29
1.3341	2	$\bar{7}12$	70.53
1.3231	1	$\bar{3}51$	71.21
1.3189	<1	$\bar{1}52$	71.47
1.3120	2	243	71.90
1.3106	1	351,152	71.99

Sample

The sample was prepared by boiling a saturated aqueous solution of $MgCl_2$ and filtering off the crystals. The sample was somewhat hygroscopic.

Color

Colorless

Optical data

Biaxial (+), N_α=1.498, N_β=1.505, N_γ=1.525. 2V is large.

Structure

Monoclinic, C2/m (12), Z = 2, isostructural with $MgBr_2 \cdot 6H_2O$. The structure of bischofite was determined by Andress and Gundermann [1934].

NBS lattice constants:

a = 9.871(2)Å
b = 7.113(1)
c = 6.079(1)
β = 93.74(1)

Density

(calculated) 1.585 g/cm^3

Reference intensity

$I/I_{corundum} \approx 0.8$

Additional patterns

1. PDF card 1-431 [Hanawalt et al., 1938].

References

Andress, K.R. and Gundermann, J. (1934). Z. Krist. 87A, 345.

Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.77	17	110	15.34
4.263	20	$\bar{1}11$	20.82
4.101	100	111	21.65
3.955	30	$\bar{2}01$	22.46
3.708	10	201	23.98
3.556	30	020	25.02
3.068	2	021	29.08
3.032	5	002	29.43
2.981	35	310	29.95
2.883	65	220	30.99
2.740	35	$\bar{3}11$	32.66
2.728	55	$\bar{1}12$	32.80
2.661	8	$\bar{2}02$	33.65
2.643	90	$\bar{2}21$,112	33.89
2.616	7	311	34.25
2.567	9	221	34.92
2.463	7	400	36.45
2.336	9	$\bar{4}01$	38.50
2.308	25	022,130	38.99
2.232	30	401	40.38
2.192	2	$\bar{3}12$	41.15
2.167	5	$\bar{1}31$	41.65
2.145	8	131	42.10
2.131	3	$\bar{2}22$	42.39
2.065	8	312	43.80
2.051	11	222	44.11
1.952	2	$\bar{4}21$	46.49
1.922	5	330	47.25
1.914	7	$\bar{2}03$	47.46
1.890	6	421	48.10
1.849	35	$\bar{1}32$	49.25
1.844	20	$\bar{5}11$	49.38
1.830	6	203	49.79
1.812	7	331	50.32
1.778	15	040	51.35
1.757	5	023	52.00
1.7272	13	$\bar{4}22$	52.97
1.7218	11	$\bar{3}13$	53.15
1.6860	4	$\bar{2}23$	54.37
1.6418	3	600	55.96
1.6221	6	$\bar{2}41$	56.70
1.5964	5	332	57.70
1.5088	4	133	61.40
1.4874	12	$\bar{5}31$	62.38

Manganese chloride hydrate, $MnCl_2 \cdot 2H_2O$

Sample

The sample was prepared by heating a solution of $MnCl_2 \cdot 4H_2O$ in ethyl alcohol. Excess alcohol was removed by pressing between filter papers.

Color

Light pink

Optical data

Biaxial (+), N_α=1.583, N_β=1.613, N_γ=1.664; 2V is very large.

Structure

Monoclinic, C2/m (12), Z=2 [Neuhaus, 1937], isostructural with $CoCl_2 \cdot 2H_2O$. The structure was determined by Vainshtein [1952].

NBS lattice constants:

a = 7.4062(5) Å
b = 8.8032(5)
c = 3.6881(5)
β = 98.22(1)°

Density

(calculated) 2.259 g/cm³

Reference intensity

$I/I_{corundum}$ = 2.3

Additional patterns

1. PDF card 1-199 [Hanawalt et al., 1938].
2. PDF card 3-743 [Neuhaus, 1937].

References

Hanawalt, J.D., Rinn, H.W.,and Frevel, L.K.(1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

Neuhaus, A. (1937). Z. Krist. 98, 112.

Vainshtein, B.K. (1952). Dokl. Akad. Nauk SSSR 83, 227.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.636	100	110	15.71
4.399	65	020	20.17
3.667	3	200	24.25
3.227	4	$\bar{1}11$	27.62
2.922	25	111	30.57
2.817	30	$\bar{2}20$	31.74
2.794	45	$\bar{2}01$	32.01
2.725	14	130	32.84
2.419	25	$\bar{2}01$	37.13
2.355	16	$\bar{2}21$,310	38.19
2.202	19	040	40.96
2.130	13	131	42.41
2.120	20	$\bar{2}21$	42.61
2.116	18	$\bar{3}11$	42.70
1.887	1	240	48.19
1.878	2	330	48.43
1.866	2	311	48.75
1.833	9	400	49.71
1.8250	8	002	49.92
1.7945	7	$\bar{1}12$	50.84
1.7499	4	$\bar{3}31$	52.23
1.7287	9	$\bar{2}41$	52.92
1.7120	2	150	53.48
1.6918	5	420	54.17
1.6282	9	241	56.48
1.6004	<1	$\bar{3}31$	57.54
1.5547	3	$\bar{1}32$	59.40
1.5304	2	151	60.44
1.4673	1	060	63.33
1.4463	1	510	64.36
1.4285	1	350	65.25
1.4084	6	$\bar{4}40$	66.31
1.3695	2	$\bar{3}51$	68.45
1.3618	1	260,061	68.89
1.3116	<1	530	71.93
1.2988	1	$\bar{2}61$	72.75
1.2841	1	511	73.72
1.2545	1	261	75.76
1.2393	1	$\bar{1}70$	76.86
1.2118	1	$\bar{6}01$	78.94
1.2096	1	402	79.11
1.1867	<1	531	80.95
1.1771	1	$\bar{6}20$	81.75
1.1682	3	$\bar{6}21$	82.50
1.1654	2	171	82.75
1.1453	2	$\bar{4}60$	84.53
1.1363	1	$\bar{5}32$	85.36
1.1266	<1	550	86.27
1.1181	1	$\bar{3}70$	87.09
1.1116	1	601,$\bar{5}51$	87.73
1.1002	<1	080	88.87
1.0893	1	$\bar{3}71$	90.00
1.0777	<1	621	91.24
1.0658	1	$\bar{4}61$	92.56
1.0615	1	$\bar{6}41$	93.05
1.0396	<1	710,$\bar{7}11$	95.62
1.0372	1	$\bar{1}72$	95.92
1.0239	<1	$\bar{2}81$	97.58
1.0096	1	$\bar{5}52$	99.45
0.9923	1	$\bar{6}41$	101.84
.9862	<1	730,$\bar{7}31$	102.71

Mercury ammine chloride, $Hg(NH_3)_2Cl_2$

Sample

The sample was prepared by exposing finely ground $HgCl_2$ to NH_3 gas in a previously evacuated desiccator.

Color

Colorless

Structure

Cubic, Z=1/2, structure determined by MacGillavry and Bijvoet [1936].

NBS lattice constant:

a = 4.053(2) Å

Density

(calculated) 3.809 g/cm^3

Reference intensity

$I/I_{corundum}$ = 1.6

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
2.868	17	110	31.16
2.342	100	111	38.41
2.028	70	200	44.65
1.4332	25	220	65.02
1.2220	19	311	78.15
1.1699	8	222	82.36

Additional patterns

1. MacGillavry and Bijvoet [1936]

References

MacGillavry, C. H. and Bijvoet, J. M. (1936). Z. Krist. **94**, 231.

Sample

The sample was made by I. Mayer [Hebrew University, Jerusalem]. A mixture of $(NH_4)_2HPO_4$ and Nd_2O_3 was heated at 500 °C for 2 hours, then at 1100 °C overnight.

Color

Pale purplish pink

Structure

Monoclinic, $P2_1/n$ (14), Z=4, isostructural with monazite. The structure of $NdPO_4$ was determined by Mooney [1948].

NBS lattice constants:
a = 6.7441(6) Å
b = 6.9584(7)
c = 6.4111(7)
β = 103.67(1)°

Density

(calculated) 5.435 g/cm³

Reference intensity

$I/I_{corundum} = 1.0$

Polymorphism

$NdPO_4$ occurs also in a low temperature modification, which may require some zeolite water for stabilization [Mooney, 1950]. PDF card 4-644 is of this form.

Additional patterns

1. Weigel et al. [1965]

References

Mooney, R.C.L. (1948). J. Chem. Phys. **16**, 1003.
Mooney, R.C.L. (1950). Acta Cryst. 3, 337.
Weigel, von F., Sherer, V. and Henschel, H. (1965) Radiochimica Acta **4**, 18.

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.17	14	$\bar{1}01$	17.13
4.78	10	110	18.56
4.645	25	011	19.09
4.151	45	$\bar{1}11$	21.39
4.064	16	101	21.85
3.508	19	111	25.37
3.479	18	020	25.58
3.277	60	200	27.19
3.116	8	002	28.62
3.072	100	120	29.04
3.040	7	021	29.36
2.965	17	$\bar{2}10$	30.12
2.933	5	$\bar{2}11$	30.45
2.842	100	012,$\bar{1}12$	31.45
2.583	25	$\bar{2}02$	34.70
2.479	<1	211	36.21
2.423	25	112,$\bar{2}12$	37.08
2.385	7	220	37.68
2.368	2	$\bar{2}21$	37.97
2.321	6	022,$\bar{1}22$	38.77
2.233	3	$\bar{3}01$	40.36
2.187	3	130	41.24
2.174	25	031	41.51
2.129	40	$\bar{1}03$	42.43
2.126	40	$\bar{3}11$	42.48
2.109	25	221	42.84
2.085	3	310	43.36
2.075	3	122,$\bar{2}22$	43.58
2.038	1	$\bar{1}13$	44.42
2.015	2	131	44.95
1.991	<1	013	45.53
1.949	35	212	46.55
1.924	9	301	47.19
1.892	1	230	48.04
1.885	16	$\bar{2}31$	48.25
1.860	35	032,$\bar{1}32$	48.93
1.851	19	$\bar{3}20$	49.19
1.8165	2	$\bar{1}23$	50.18
1.7945	2	113	50.84
1.7834	11	023	51.18
1.7521	20	$\bar{3}22$	52.16
1.7400	7	040	52.55
1.7266	25	132,$\bar{2}32$	52.99
1.7215	20	$\bar{3}03$	53.16
1.6812	12	140	54.54
1.6715	1	$\bar{3}13$	54.88
1.6494	1	$\bar{1}41$	55.68
1.6383	6	123,400	56.09
1.6159	9	$\bar{4}02$	56.94
1.5989	2	141	57.60

d (Å)	I	hkl	2θ(°)
1.5949	9	410	57.76
1.5903	8	330	57.94
1.5757	5	312	58.53
1.5616	3	114	59.11
1.5573	6	004,204	59.29
1.5427	<1	323	59.91
1.5364	3	240	60.18
1.5267	6	332	60.60
1.5193	13	214,042	60.93
1.4820	<1	420	62.63
1.4659	3	411,422	63.40
1.4554	6	124,241	63.91
1.4477	4	223	64.29
1.4431	4	142,242	64.52
1.4214	1	024,224	65.63
1.4092	3	314	66.27
1.3768	4	421	68.04
1.3636	5	431	68.79
1.3605	5	150,340	68.97
1.3534	2	303	69.38
1.3507	3	423	69.54
1.3470	3	143	69.76
1.3436	3	151	69.96
1.3332	5	043	70.59
1.3292	11	324,313	70.83
1.3270	13	332,402	70.97
1.3237	6	511	71.17
1.3200	8	342	71.40
1.3187	8	134	71.48
1.3125	2	233	71.87
1.3063	2	243	72.27
1.3030	5	412	72.48
1.2927	5	034,234,+	73.15
1.2880	3	510	73.46
1.2805	2	250,105	73.96
1.2701	12	152,414,+	74.67
1.2595	4	115,431	75.41
1.2495	2	503	76.12
1.2382	6	522	76.94
1.2300	<1	513	77.55
1.2254	8	501,152	77.89
1.2228	12	334	78.09
1.2123	2	224	78.90

Nickel chloride hydrate, $NiCl_2 \cdot 6H_2O$

Sample

The sample was prepared by slow evaporation at room temperature of an aqueous solution of $NiCl_2$ (Fisher Scientific Co.). Because of the platy nature and the instability of the material, the intensity values are subject to some error.

Color

Deep yellowish green

Optical data

Biaxial (+) N_α=1.590, N_β=1.620, N_γ=1.648; 2V is very large.

Structure

Monoclinic, I2/m (12), Z = 2, isostructural with $CoCl_2 \cdot 6H_2O$. The structure was determined by Mizuno (1961).

NBS lattice constants:

a = 8.786(2)Å
b = 7.076(2)
c = 6.625(2)
β = 97.21(1)°

Density

(calculated) 1.932 g/cm³

Additional patterns

1. PDF card 1-200 [Hanawalt et al., 1938]

References

Hanawalt, J.D., Rinn, R.W., and Frevel, L.K.(1938). Ind. Eng. Chem. Anal. Ed. **10**, 457.

Mizuno, J. (1961). J. Phys. Soc. Japan **16**, 1574.

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.59	100	$\bar{1}01$	15.83
5.50	40	110	16.10
4.96	12	101	17.88
4.82	35	011	18.39
4.360	2	200	20.35
3.542	10	020	25.12
3.392	2	$\bar{2}11$	26.25
3.288	1	002	27.10
3.095	4	211	28.82
2.994	9	$\bar{1}21$	29.82
2.926	35	$\bar{1}12$	30.53
2.799	17	$\bar{2}02$	31.95
2.747	30	220	32.57
2.729	5	112	32.79
2.689	20	310	33.29
2.543	8	301	35.27
2.407	16	022	37.32
2.220	3	031	40.60
2.211	2	$\bar{3}12$	40.77
2.192	5	$\bar{1}03,\bar{3}21$	41.14
2.178	20	400	41.42
2.065	3	103,321	43.81
2.057	7	411	43.98
2.030	4	222	44.59
2.013	1	$\bar{2}31$	45.00
1.980	3	$\bar{2}13$	45.80
1.971	8	312	46.00
1.932	3	$\bar{4}02$	47.00
1.921	3	411	47.29
1.900	10	$\bar{1}32$	47.83
1.862	5	$\bar{1}23$	48.85
1.856	5	420	49.03
1.832	2	330	49.74
1.783	1	123	51.20
1.695	7	$\bar{4}22$	54.07
1.687	3	$\bar{1}41$	54.35
1.636	1	501	56.17
1.6084	3	$\bar{1}14,\bar{4}13$	57.23
1.6045	6	$\bar{2}04$,033	57.38
1.5888	3	$\bar{4}31$	58.00
1.5853	3	$\bar{5}12$	58.14
1.5609	2	$\bar{5}21$	59.14
1.5575	2	042	59.28
1.5483	4	332	59.67
1.4969	2	323	61.94
1.4774	1	204	62.85
1.4628	2	233,$\bar{2}24$	63.55
1.4558	2	$\bar{5}03$	63.89
1.4514	2	341	64.11

Nickel fluoride hydrate, $NiF_2 \cdot 4H_2O$

Sample
The sample was made by slow evaporation at room temperature of an aqueous solution of NiF_2 with a slight excess of HF.

Color
Brilliant yellow green

Structure
Orthorhombic, $P2_1ab$ (29), Z=4, isostructural with $ZnF_2 \cdot 4H_2O$. The space group and cell parameters of $ZnF_2 \cdot 4H_2O$ were determined by Rao et al. [1965].

NBS lattice constants:
a = 7.485(2)Å
b = 12.482(2)
c = 5.272(1)

Density
(calculated) 2.276 g/cm^3

Reference intensity
$I/I_{corundum}$ 2.0

Polymorphism
Easwaran and Srinivasan [1965] reported, by comparison of powder patterns, that $NiF_2 \cdot 4H_2O$ was isostructural with $FeF_2 \cdot 4H_2O$. However, Penfold and Taylor [1960] reported $FeF_2.4H_2O$ as rhombohedral. This suggests a second form of $NiF_2 \cdot 4H_2O$ exists.

Additional patterns
1. PDF card 1-267 [Hanawalt et al., 1938]

References

Easwaran, K.R.K. and Srinivasan, R. (1965). Proc. Nuclear Physics - Solid State Physics Symposium, Calcutta, Part A, 171.

Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. **10**, 457.

Penfold, B.R. and Taylor, M.R. (1960). Acta Cryst. **13**, 953.

Rao, K.V.K., Naidu, S.V.N., and Rao, P.V. (1965). Indian J. Pure Applied Phys. **3**, 68.

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.28	6	001	16.78
4.857	85	011	18.25
4.795	100	120	18.49
4.075	50	111	21.79
3.748	6	200	23.73
3.546	3	121	25.09
3.266	3	031	27.28
3.120	30	040	28.59
3.052	4	201	29.24
2.964	35	211	30.13
2.741	15	221	32.64
2.637	1	002	33.97
2.580	3	012	34.74
2.528	8	141	35.48
2.460	3	231	36.49
2.439	6	112	36.82
2.309	4	122	38.98
2.256	1	051	39.93
2.219	8	311	40.62
2.155	25	202	41.89
2.124	4	212	42.53
2.037	1	222	44.43
2.004	13	160	45.22
1.982	3	331	45.74
1.933	9	251	46.98
1.913	3	232	47.49
1.871	5	400	48.61
1.828	1	341	49.85
1.793	5	312,420	50.90
1.773	10	242	51.51
1.740	13	013,322	52.56
1.719	1	261	53.24
1.689	2	071	54.25
1.674	1	351	54.81
1.661	2	332	55.25
1.648	4	171	55.72
1.6311	3	252	56.36
1.6050	2	440	57.36
1.5974	3	360	57.66
1.5951	2	162	57.75
1.5821	2	133	58.27
1.5787	1	213	58.41
1.5607	1	080	59.15

Potassium bromide iodide, $KBr_{.33}I_{.67}$

Sample
The sample was prepared by melting a 1:2 mixture of KBr and KI. After grinding, it was annealed at 450 °C overnight.

Color
Colorless

Optical data
Isotropic, N=1.633

Structure
Cubic, Fm3m (225), Z = 4, NaCl type. There is a complete solid solution series from KBr to KI [Wrzesnewsky, 1912].

NBS lattice constant:
a = 6.9174(3)Å

Density
(calculated) 3.02 g/cm^3

Reference intensity
$I/I_{corundum} = 8.4$

References
Wrzesnewsky, J.B. (1912). Z. anorg. Chem. **74**, 110.

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
3.997	25	111	22.22
3.456	100	200	25.76
2.446	40	220	36.71
2.086	10	311	43.35
1.997	10	222	45.37
1.7290	7	400	52.91
1.5868	2	331	58.08
1.5464	10	420	59.75
1.4118	5	422	66.13
1.3312	1	511	70.71
1.2227	1	440	78.10
1.1694	1	531	82.40
1.1528	2	600	83.85
1.0935	1	620	89.56
1.0549	<1	533	93.81
1.0428	<1	622	95.24
.9985	<1	444	100.96
.9687	<1	711	105.34
.9592	<1	640	106.85
.9245	<1	642	112.85
.9006	<1	731	117.58
.8388	<1	800	133.34

Potassium bromide iodide, $KBr_{.67}I_{.33}$

Sample
The sample was prepared by melting together KBr and KI in a 2:1 molar ratio. After grinding the sample was heated at 400 °C overnight.

Color
Colorless

Structure
Cubic, Fm3m (225), Z = 4, NaCl type. There is a complete solid solution series between KBr and KI [Wrzesnewsky, 1912].

NBS lattice constant:
a = 6.7624(3)Å

Density
(calculated) 2.90 g/cm^3

Reference intensity
$I/I_{corundum}$ = 8.4.

Optical data
Isotropic, N=1.597

References
Wrzesnewsky, J.B. (1912). Z. anorg. Chem. 74, 110.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
3.909	15	111	22.73
3.380	100	200	26.35
2.390	30	220	37.60
2.040	5	311	44.38
1.952	7	222	46.48
1.691	5	400	54.19
1.5514	2	331	59.54
1.5125	7	420	61.23
1.3805	3	422	67.83
1.3014	1	511	72.58
1.1959	1	440	80.20
1.1431	<1	531	84.73
1.1273	1	600	86.20
1.0693	1	620	92.17
1.0193	<1	622	98.17
.9760	<1	444	104.22
.9467	<1	711	108.90
.9377	<1	640	110.46
.9036	<1	642	116.97
.8805	<1	731	122.04
.8453	<1	800	131.36
.8200	<1	820	139.88

Potassium cobalt fluoride, K_2CoF_4

Sample

The sample was prepared by treating a 1:1 mixture of K_2CO_3 and $CoCO_3$ with HF, drying, and heating the product for 10 minutes at 400 °C, followed by 10 minutes at 750 °C.

Color

Medium pink

Structure

Tetragonal, I4/mmm (139), Z=2, isostructural with K_2MgF_4 and similar tetrafluorides [Rüdorff et al., 1959]. The structure of K_2MgF_4 was determined by Brehler and Winkler [1954].

NBS lattice constants:

a = 4.0750(4)Å
c = 13.089(1)

Density

(calculated) 3.256 g/cm^3

Reference intensity

$I/I_{corundum}$ 3.4

Major impurities

∿ .05% Ag, Ca, Cu, Fe, Ni, Zn and Si.

∿ .5% Al

References

Brehler, B. and Winkler, H.G.F. (1954). Heidelberger Beitr. Mineral. Petrog. **4**, 6.

Rüdorff, W., Kändler, J., Lincke, G.,and Babel, D. (1959). Angew. Chem. **71**, 672.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
6.53	100	002	13.54
3.890	8	101	22.84
3.272	1	004	27.23
2.976	40	103	30.00
2.879	30	110	31.04
2.637	2	112	33.97
2.202	10	105	40.95
2.181	40	006	41.36
2.163	10	114	41.72
2.038	25	200	44.42
1.946	3	202	46.64
1.806	1	211	50.49
1.7394	7	116	52.57
1.6814	8	213	54.53
1.6364	5	008	56.16
1.4956	3	215	62.00
1.4891	9	206	62.30
1.4403	4	220	64.66
1.4229	1	118	65.55
1.3697	1	109	68.44
1.3089	<1	0·0·10	72.10
1.2970	1	303	72.87
1.2884	2	310	73.43
1.2756	2	208	74.29
1.2058	1	305	79.41
1.2022	2	226	79.69
1.1919	1	1·1·10	80.52
1.1421	1	1·0·11	84.82
1.1365	1	219	85.34
1.1097	1	316	87.92

Potassium tungsten oxide, K_2WO_4

Sample

The sample was prepared by adding KOH solution to an aqueous solution of H_2WO_4.

Color

Colorless

Structure

Monoclinic, C2/m (12), Z = 4. The structure was determined by Koster et al. (1969).

NBS lattice constants:

a = 12.383(1)Å
b = 6.1194(8)
c = 7.5526(9)
β = 115.95(1)°

Density

(calculated) 4.208 g/cm^3

Polymorphism

K_2WO_4 undergoes a transition at 370 °C [Schmitz-Dumont and Weeg, 1951]

Additional patterns

1. PDF card 19-1004 [Gelsing et al., 1965]
2. PDF card 21-703 [Hatterer et al., 1968]
3. Kools et al. [1970]

References

Gelsing, R. J. H., Stein, H. N., and Stevels, J.M. (1965). Rec. Trav. Chim. **84**, 1452.

Hatterer, A., Kessler, H., and Ringenbach, C. (1968). Compt. Rend. Paris **266C**, 328.

Kools, F. X. N. M., Koster, A. S., and Rieck, G.D. (1970). Acta Cryst. **B26**, 1974.

Koster, A.S., Kools, F. X. N. M., and Rieck, G.D. (1969). Acta Cryst. **B25**, 1704.

Schmitz-Dumont, O. and Weeg, A. (1951). Z. Anorg. Chem. 265, 139.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
6.80	8	001	13.00
5.70	50	$\bar{2}01$	15.52
5.566	30	200	15.91
5.365	30	$1\bar{1}0$	16.51
4.719	90	$\bar{1}11$	18.79
3.834	45	$1\bar{1}1$	23.18
3.708	25	$\bar{2}02$	23.98
3.601	25	201	24.70
3.397	85	002	26.21
3.173	100	310	28.10
3.092	19	$\bar{4}01$	28.85
3.059	60	020	29.17
2.928	60	$\bar{3}12$	30.51
2.848	4	$\bar{4}02$	31.38
2.784	14	400	32.12
2.696	9	$\bar{2}21$	33.20
2.683	7	220	33.37
2.630	6	$1\bar{1}2$	34.06
2.359	6	$\bar{2}22$	38.11
2.332	13	221	38.57
2.324	9	$\bar{4}03$	38.71
2.293	17	$\bar{3}13$	39.26
2.273	45	022	39.62
2.253	12	$40\bar{1}$	39.98
2.240	11	$\bar{5}12$	40.22
2.176	5	$\bar{4}21$	41.46
2.092	3	$5\bar{1}0$	43.22
2.048	11	$\bar{6}02$	44.18
2.030	4	$\bar{6}01$	44.59
2.006	2	130	45.17
1.978	25	$31\bar{2}$	45.83
1.967	10	$\bar{1}31$	46.10
1.944	5	$113,\bar{2}23$	46.69
1.899	6	$\bar{6}03$	47.85
1.885	5	131	48.25
1.868	4	$\bar{2}04$	48.71
1.855	11	$600,\bar{4}04$	49.07
1.849	12	$\bar{4}23$	49.23
1.835	2	203	49.63
1.814	8	421	50.26
1.804	16	$\bar{3}14$	50.56
1.788	14	330	51.04
1.740	9	$\bar{3}32$	52.55
1.706	11	$\bar{5}14$	53.69
1.702	13	$\bar{6}22$	53.82

d (Å)	I	hkl	2θ(°)
1.6984	10	$\bar{7}12$,004	53.94
1.6671	3	$\bar{6}04$	55.04
1.6607	6	$\bar{7}11$	55.27
1.6351	3	$\bar{7}13$	56.21
1.6133	3	$\bar{6}23$	57.04
1.5946	6	$\bar{2}24$	57.77
1.5866	9	620,$\bar{4}24$	58.09
1.5742	6	223,$\bar{3}33$	58.59
1.5559	4	$\bar{5}32$	59.35
1.5514	4	422	59.54
1.5474	3	$\bar{8}02$	59.71
1.5293	7	040,114	60.49
1.5043	2	530	61.60
1.4846	5	024	62.51
1.4649	8	$\bar{6}24$	63.45
1.4620	11	$\bar{3}15$	63.59
1.4601	8	332	63.68
1.3854	6	$\bar{3}34$,531	67.56
1.3803	5	$\bar{8}22$,711	67.84
1.3715	2	$\bar{4}41$	68.34
1.3384	5	$\bar{9}12$,$\bar{7}15$	70.27
1.3337	4	$\bar{9}13$	70.56
1.3075	4	314,$\bar{2}43$	72.19
1.3000	3	$\bar{6}25$	72.67

Sodium bromide chloride, $NaBr_{.33}Cl_{.67}$

Sample
The sample was prepared by melting a 1:2 mixture of NaBr and NaCl. After grinding it was annealed for 18 hours at 600 °C in a sealed glass tube.

Color
Colorless

Optical data
Isotropic, N=1.577

Structure
Cubic, Fm3m (225), Z=4. There is a complete solid solution between NaBr and NaCl [Gromakov and Gromakova, 1955].

NBS lattice constant:
a = 5.7614(2)Å

Density
(calculated) 2.54 g/cm^3

Reference intensity
$I/I_{corundum}$ = 4.2

Reference
Gromakov, S.P. and Gromakova, L.M. (1955). Zh.Fiz. Khim. 29, 746.

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ (°)
3.329	30	111	26.76
2.882	100	200	31.00
2.037	45	220	44.43
1.7373	6	311	52.64
1.6632	11	222	55.18
1.4401	5	400	64.67
1.3216	2	331	71.30
1.2883	9	420	73.44
1.1761	5	422	81.83
1.1089	1	511	88.00
1.0185	1	440	98.28
0.9739	<1	531	104.54
.9603	1	600	106.67
.9108	1	620	115.49
.8686	1	622	124.95
.8317	<1	444	135.68
.8067	<1	711	145.43
.7990	<1	640	149.18

Sodium bromide chloride, $NaBr_{.67}Cl_{.33}$

Sample

The sample was prepared by melting a 2:1 mixture of NaBr and NaCl. After grinding it was annealed for 18 hours at 600 °C in a sealed glass tube.

Color

Colorless

Optical data

Isotropic, N = 1.610

Structure

Cubic, Fm3m (225), Z=4. There is a complete solid solution series between NaBr and NaCl [Gromakov and Gromakova, 1955].

NBS lattice constant:
a = 5.8676(2)Å

Density

(calculated) 2.87 g/cm^3

Reference intensity

$I/I_{corundum}$ = 5.5

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
3.387	60	111	26.29
2.933	100	200	30.45
2.0742	60	220	43.60
1.7692	12	311	51.62
1.6944	18	222	54.08
1.4669	6	400	63.35
1.3463	4	331	69.80
1.3121	15	420	71.90
1.1977	9	422	80.05
1.1292	3	511	86.02
1.0375	2	440	95.88
.9918	2	531	101.91
.9780	4	600	103.93
.9277	3	620	112.26
.8949	<1	533	118.80
.8846	2	622	121.09
.8216	<1	711	139.28
.8136	1	640	142.42

References

Gromakov, S. P. and Gromakova, L. M. (1955). Zh. Fiz. Khim. 29, 746.

Sodium carbonate sulfate, $Na_4CO_3SO_4$

Sample

The sample was prepared by melting together equal molar amounts of Na_2CO_3 and Na_2SO_4.

Major impurities

∿ .05% Ag, Al, Ca, K and Si.

Color

Colorless

Optical data

Uniaxial (-), N ≅ 1.45

Structure

Hexagonal, $P\bar{3}ml$ (164), Z=1, isostructural with Na_2SO_4, form I, and with α-Na_2CO_3. A continuous isomorphous series exists in all proportions from zero to 75 mol. percent Na_2CO_3 [Schroeder et al., 1936]. The structure of this type of compound was determined by Gossner [1928].

NBS lattice constants:

a = 5.2284(5) Å
c = 6.8808(8)

Density

(calculated) 2.528 g/cm^3

Reference intensity

$I/I_{corundum}$ = 1.1

Polymorphism

The 1:1 composition may occur in several other crystal forms [Khlapova and Kovaleva, 1963].

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.528	7	100	19.59
3.783	60	101	23.50
3.440	45	002	25.88
2.741	100	102	32.64
2.614	70	110	34.28
2.263	2	200	39.80
2.150	14	201	41.98
1.891	35	202	48.07
1.720	8	004	53.20
1.710	4	210	53.53
1.611	1	203	57.14
1.5322	9	212	60.36
1.5094	6	300	61.37
1.4366	8	114	64.85
1.3825	1	302	67.72
1.3722	1	213	68.30
1.3166	1	105	71.61
1.3073	6	220	72.20
1.2218	5	222	78.17
1.1796	3	312	81.54
1.1467	1	006	84.40
1.1347	3	304	85.51
1.1119	1	106	87.70
1.1016	1	313	88.73
1.0753	2	402	91.51
1.0407	2	224	95.49

References

Gossner, B. (1928). Neues Jahrb. Mineral. Geol., Beilage Bd. 57A, 89.

Khlapova, A. N. and Kovaleva, E. S. (1963). J. Struct. Chem. USSR (Eng. Transl.) **4**, 517.

Schroeder, W.C., Berk, A.A., Partridge, E.P., and Gabriel, A. (1936). J. Am. Chem. Soc. 58, 846.

Sodium carbonate sulfate (burkeite), $Na_6CO_3(SO_4)_2$

Sample

The sample was precipitated by mixing boiling aqueous solutions of Na_2CO_3 and Na_2SO_4 in a molar ratio of 1:2. Chemical analysis of the precipitate indicated a ratio of 1:2.0.

Color

Colorless

Structure

Orthorhombic, Z=4/3. Ramsdell [1942] reported a cell with the a and b parameters tripled. No evidence was seen here for an enlarged cell. This phase occurs over a range of solid solution [Caspari, 1924] [Schroeder et al., 1936]. Khlapova and Burovaya [1957] reported that this phase ("rhombic" burkeite) contained essential H_2O. However the weight loss found at NBS between 350 and 700 °C was only 0.32% after the material had been transformed to the hexagonal form of the α-Na_2SO_4 type.

NBS lattice constants:

a = 7.055(2) Å
b = 9.215(2)
c = 5.167(1)

Density

(calculated) 2.571 g/cm^3

Reference intensity

$I/I_{corundum} = 0.7$

Polymorphism

In studies of the system Na_2CO_3-Na_2SO_4 Khlapova and Burovaya [1957] and Khlapova and Kovaleva [1963] found three hexagonal polymorphs of the 1:2 composition, not including this one which they considered a hydrate. Transitions were reported to occur at 400 and 575 °C.

Additional patterns

1. PDF card 2-840 [Michigan Alkali Co. Wyandotte Michigan].
2. Ramsdell [1939].

References

Caspari, W. A. (1924). J. Chem. Soc. 125, 2381.
Khlapova, A.N. and Burovaya, E.E. (1957). Russ. J. Inorg. Chem. (English Transl.) **2**, No.8, 249.
Khlapova, A. N. and Kovaleva, E. S. (1963). J. Struct. Chem. USSR (Eng. Transl.) **4**, 517.
Ramsdell, L.S. (1939). Am. Mineralogist **24**, 109.
Ramsdell, L.S. (1942). Am. Mineralogist **27**, 230.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
9.215	8	010	9.59
4.607	5	020	19.25
4.507	17	011	19.68
4.172	4	101	21.28
3.854	40	120	23.06
3.795	75	111	23.42
3.526	80	200	25.24
3.439	19	021	25.89
3.307	3	210	26.99
3.072	17	030	29.04
2.801	100	220	31.93
2.777	55	211	32.21
2.640	75	031	33.93
2.583	75	002	34.70
2.488	5	012	36.07
2.345	6	112	38.35
2.305	11	040	39.05
2.279	4	310	39.51
2.191	3	140	41.17
2.147	14	122	42.04
2.142	11	301	42.15
2.105	6	041	42.94
1.978	12	032	45.84
1.929	30	240	47.07
1.904	25	132	47.74
1.898	30	222	47.88
1.784	2	150	51.17
1.764	17	400	51.79
1.735	8	051	52.71
1.722	3	003	53.15
1.673	2	103	54.83
1.645	3	113,340+	55.85
1.635	4	250	56.20
1.627	4	322	56.53
1.614	4	023	57.00
1.557	5	251	59.30
1.548	6	203	59.67
1.545	5	242	59.82
1.536	6	060	60.20
1.526	5	213	60.64
1.503	6	033	61.67

Sodium carbonate sulfate, $Na_6CO_3(SO_4)_2$

Sample

The sample was prepared by melting a 1:2 molar mixture of Na_2CO_3 and Na_2SO_4. The sample was somewhat hygroscopic.

Color

Colorless

Structure

Hexagonal, $P\bar{3}m1$ (164), $Z=\frac{2}{3}$, isostructural with Na_2SO_4, form I, and with α-Na_2CO_3. A continuous series of isomorphous phases occurs in all proportions from zero to 75 mol. percent of Na_2CO_3 [Schroeder et al., 1936]. The structure of this type of compound was determined by Gossner [1928].

NBS lattice constants:

a = 5.2624(4) Å

c = 7.0236(7)

Density

(calculated) 2.563 g/cm^3

Reference intensity

$I/I_{corundum} = 1.1$

Polymorphism

This composition may occur in several other crystal forms [Khlapova and Kovaleva, 1963].

References

Gossner, B. (1928). Neues Jahrb. Mineral. Geol., Beilage Bd. 57A, 89.

Khlapova, A. N. and Kovaleva, E. S. (1963). J. Struct. Chem. USSR (Eng. Transl.) **4**, 517.

Schroeder, W.C., Berk, A.A., Partridge, E.P., and Gabriel, A. (1936). J. Am. Chem. Soc. **58**, 846.

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.558	10	100	19.46
3.824	85	101	23.24
3.515	50	002	25.32
2.783	100	102	32.14
2.631	80	110	34.05
2.279	4	200	39.51
2.167	11	201	41.65
2.106	1	112	42.90
1.912	40	202	47.51
1.755	10	004	52.06
1.7227	3	210	53.12
1.6332	2	203	56.28
1.5471	11	212	59.72
1.5190	7	300	60.94
1.4848	1	301	62.50
1.4603	10	114	63.67
1.3949	2	302	67.04
1.3876	2	213	67.44
1.3424	1	105	70.03
1.3154	5	220	71.69
1.2639	1	310	75.10
1.2439	1	311	76.52
1.2318	2	222	77.41
1.1892	3	312	80.74
1.1706	1	006	82.30
1.1488	4	304	84.21
1.1337	2	106	85.60
1.1121	2	313	87.68
1.0887	<1	215	90.07
1.0837	2	402	90.60
1.0529	2	224	94.04
1.0409	<1	206	95.47

Sodium carbonate sulfate, $Na_6(CO_3)_2SO_4$

Sample

The sample was prepared by melting Na_2CO_3 and and Na_2SO_4 together in a 2:1 molar ratio.

Major impurities

∿ .05% Ca

Color

Colorless

Structure

Hexagonal, $P\bar{3}ml$ (164), $Z=\frac{2}{3}$, isostructural with Na_2SO_4, form I, and with α-Na_2CO_3. A continuous isomorphous series exists in all proportions from zero to 75 mol. percent Na_2CO_3 [Schroeder et al., 1936]. The structure of this type of compound was determined by Gossner [1928].

NBS lattice constants:

a = 5.2034(5)Å

c = 6.683(1)

Density

(calculated) 2.501 g/cm^3

Reference intensity

$I/I_{corundum} = 0.7$

Polymorphism

This composition may occur in several other crystal forms [Khlapova and Kovaleva, 1963].

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.505	4	100	19.69
3.739	45	101	23.78
3.341	55	002	26.66
2.684	100	102	33.35
2.603	75	110	34.43
2.253	2	200	39.99
2.135	25	201	42.29
1.868	35	202	48.72
1.7034	5	210	53.77
1.6707	6	004	54.91
1.6508	2	211	55.63
1.5836	2	203	58.21
1.5181	6	212	60.98
1.5019	6	300	61.71
1.4655	1	301	63.42
1.4062	4	114	66.43
1.3527	1	213	69.42
1.3008	5	220	72.62
1.2814	<1	105	73.90
1.2453	1	303	76.42
1.2125	3	222	78.88
1.1706	3	312	82.30

References

Gossner, B. (1928). Neues Jahrb. Mineral. Geol., Beilage Bd. 57A, 89.

Khlapova, A. N. and Kovaleva, E. S. (1963). J. Struct. Chem. USSR (Eng. Transl.) 4, 517.

Schroeder, W.C., Berk, A.A., Partridge, E.P., and Gabriel, A. (1936). J. Am. Chem. Soc. **58**, 846.

Sample

The sample was prepared by melting an equimolar mixture of Na_2SO_4 and Na_2CrO_4. This material was then annealed for 18 hours at 600 °C, followed by 350 °C for 2 hours in a stream of oxygen.

Color

Brilliant greenish yellow

Structure

Orthorhombic, Amam (63), Z=2, isostructural with Na_2CrO_4 and Na_2SO_4 (III) [Fischmeister,1954]. The structure of Na_2CrO_4 was determined by Miller [1936], and the space group was corrected by Niggli [1954]. Na_2CrO_4 and Na_2SO_4(III) form a complete isomorphous series [Fischmeister,1954].

NBS lattice constants:

a = 7.055(2)Å
b = 9.115(2)
c = 5.744(2)

Density

(calculated) 2.733 g/cm³

Reference intensity

$I/I_{corundum}$ = 0.8

Major impurities

∿ .05% Ag and Al

References

Fischmeister, H. (1954). Acta Cryst. 7, 776.
Miller, J.J. (1936). Z. Krist. 94, 131.
Niggli, A. (1954). Acta Cryst. 7, 776.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.857	15	011	18.25
4.555	3	020	19.47
4.003	50	111	22.19
3.831	45	120	23.20
3.527	55	200	25.23
2.869	75	002	31.15
2.855	100	211	31.30
2.687	60	031	33.32
2.511	2	131	35.73
2.430	20	022	36.96
2.280	3	040	39.49
2.168	2	140	41.62
2.135	6	231	42.29
2.116	3	311	42.70
2.089	7	320	43.28
2.000	16	222	45.30
1.915	9	240	47.44
1.811	2	113	50.34
1.770	10	331	51.60
1.764	20	400	51.79
1.686	1	151	54.31
1.656	4	213	55.45
1.619	8	033	56.81
1.5926	10	242	57.85
1.5585	2	251	59.24
1.5032	2	402	61.65
1.4742	10	431	63.00

Sodium magnesium carbonate (eitelite), $Na_2Mg(CO_3)_2$

Sample

The sample was made by reacting a saturated solution of sodium hydrogen carbonate with a suspension of basic magnesium carbonate.

Color

Colorless

Optical data

Uniaxial (-), N_e =1.450, N_o =1.605 [Pabst, 1973].

Structure

Hexagonal, $R\bar{3}$ (148), Z = 3 [Pabst, 1973]. Eitel and Skaliks [1929] previously reported $P\bar{3}$ (147) as the space group.

NBS lattice constants:
a = 4.9423(2)Å
c = 16.396(1)

Density (calculated) 2.792 g/cm³

Reference intensity

$I/I_{corundum}$ 1.8

Additional patterns

1. PDF card 4-737 [Wyandotte Chem. Co., Wyandotte, Michigan]

References

Eitel, W. and Skaliks, W.(1929). Z. anorg. u. allgem. Chem. 183, 263.

Pabst, A. (1973). Am. Mineralogist 58, 211.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.48	<1	003	16.17
3.794	16	012	23.43
2.731	25	006	32.77
2.602	100	015	34.44
2.469	25	110	36.36
2.251	20	113	40.03
2.121	2	021	42.58
2.0710	18	202	43.67
1.8975	20	024	47.90
1.8486	2	018	49.25
1.8333	9	116	49.69
1.7925	9	205	50.90
1.6099	8	211	57.17
1.5873	2	122	58.06
1.5311	11	1·0·10	60.41
1.5048	1	214	61.58
1.4803	1	208	62.71
1.4663	4	119	63.38
1.4505	6	125	64.15
1.4264	5	300	65.37
1.3802	<1	303	67.85
1.3665	1	0·0·12	68.62
1.3310	1	217	70.72
1.3016	<1	0·2·10	72.57
1.2695	1	128	74.71
1.2355	4	220	77.14
1.2232	<1	2·0·11	78.06
1.1957	<1	1·1·12	80.21
1.1841	1	131	81.16
1.1749	<1	312	81.93
1.1516	3	2·1·10	83.96
1.1297	<1	0·1·14	85.98
1.1233	<1	309	86.59
1.1163	4	315	87.27
1.0962	<1	1·2.11	89.29
1.0930	1	0·0.15	89.62
1.0865	<1	0·2·13	90.30
1.0588	<1	137	93.35
1.0353	<1	404	96.15
1.0271	<1	2·0·14,318	97.18
1.0227	<1	229	97.74
1.0172	1	045	98.44
0.9996	<1	1·1·15	100.82
.9947	<1	2·1·13	101.50
.9750	<1	232	104.38
.9615	1	1·3·10	106.47
.9550	<1	324	107.53
.9488	<1	1·2·14,048	108.55
.9406	1	235	109.95
.9340	1	410	111.12

Sample

The sample was prepared by heating Na_2SO_4 at 700 °C for one hour. The sample changes to Na_2SO_4, form V, if exposed to moist air.

Color

Colorless

Structure

Orthorhombic, Amam (63), Z=4, isostructural with Na_2CrO_4 [Frevel, 1940]. The structure of Na_2CrO_4 was determined by Miller [1936]. The space group was corrected by Niggli [1954].

NBS lattice constants:

a = 6.9666(9) Å
b = 8.9511(9)
c = 5.6109(6)

Density

(calculated) 2.696 g/cm^3

Reference intensity

$I/I_{corundum}$ = 1.8

Polymorphism

The polymorphism of Na_2SO_4 is complex and not completely resolved. The form reported here is stable at room temperature and has been referred to as Na_2SO_4, form III; Na_2SO_4, form I, is hexagonal and is stable above 250°C. [Kracek and Ksanda, 1930]. Khlapova [1956] reported a form (δ), stable between 600°C. and the melting point (900°C.). Khlapova and Burovaya [1957] discussed the phase of Na_2SO_4 known as form V and as the mineral thenardite. They considered it to be a hydrate.

Additional patterns

1. PDF card 8-31 [Fischmeister, 1954]
2. Das Gupta [1954]

References

Das Gupta, D. R. (1954). Acta Cryst. 7, 275.
Fischmeister, H. (1954). Acta Cryst. 7, 776.
Frevel, L.K. (1940). J. Chem. Phys. 8, 290.
Khlapova, A.N.(1956). Russ. J. Inorg. Chem. (English Transl.) 1, No. 11, 132.
Khlapova, A.N. and Burovaya, E.E. (1957). Russ. J. Inorg. Chem. (English Transl.) 2, No.8, 249.
Kracek, F. C. and Ksanda, C. J. (1930). J. Phys. Chem. 34, 1741.
Miller, J.J. (1936). Z. Krist. 94, 131.
Niggli, A. (1954). Acta Cryst. 7, 776.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.759	9	011	18.63
4.476	4	020	19.82
3.929	35	111	22.61
3.768	30	120	23.59
3.485	25	200	25.54
2.809	100	211,002	31.83
2.636	45	031	33.98
2.465	2	131	36.42
2.377	20	022	37.82
2.238	4	040	40.26
2.184	2	202	41.31
2.131	6	140	42.39
2.101	6	231	43.01
2.086	7	311	43.33
2.062	5	320	43.87
1.963	18	222	46.20
1.883	9	240	48.29
1.831	1	013	49.76
1.771	1	113	51.56
1.7496	13	042	52.24
1.7419	18	331,400	52.49
1.6964	2	142	54.01
1.6229	3	420	56.67
1.6206	4	213	56.76
1.6115	3	340	57.11
1.5845	9	033	58.17
1.5633	10	242	59.04
1.5320	3	251	60.37
1.4919	1	060	62.17
1.4799	2	402	62.73
1.4528	9	431	64.04
1.4425	2	233	64.55
1.4028	4	004	66.61
1.3748	3	351,440	68.15
1.3370	1	511	70.36
1.3302	2	520	70.77
1.3168	3	062	71.60
1.3144	2	124	71.75
1.2941	3	162	73.06
1.2714	2	153	74.58
1.2494	1	224	76.12
1.2317	2	262,531	77.42

Strontium chloride hydrate, $SrCl_2 \cdot 2H_2O$

Sample
The sample was prepared by heating $SrCl_2 \cdot 6H_2O$ at 60 - 70 °C for several hours under vacuum.

Color
Colorless

Structure
Monoclinic, Cc (9) or C2/c (15), Z=4. The structure was determined by Jensen [1942].

NBS lattice constant:
a = 11.688(1)Å
b = 6.4048(5)
c = 6.6957(6)
β = 105.54(1)°

Density
(calculated) 2.676 g/cm³

Reference intensity
$I/I_{corundum}$ 1.0

Additional patterns
1. PDF card 3-500 [Jensen, 1942].

References
Jensen, A.T.(1942). Kgl. Danske Videnskab. Selskab Mat. Fys. Medd. 20, Nr.5.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.63	60	200	15.74
4.523	75	$\bar{1}11$	19.61
3.964	35	111	22.41
3.238	35	310	27.52
3.229	30	002	27.60
3.206	100	$\bar{3}11$,020	27.80
2.966	4	$\bar{1}12$	30.10
2.871	20	021	31.13
2.816	2	400	31.75
2.784	45	220	32.12
2.690	30	$\bar{2}21$	33.28
2.659	75	311	33.68
2.645	40	112	33.86
2.608	20	$\bar{3}12$	34.36
2.523	35	202	35.55
2.475	30	$\bar{4}02$	36.27
2.442	14	221	36.78
2.272	30	022	39.63
2.261	35	$\bar{2}22$	39.84
2.189	13	$\bar{5}11$	41.20
2.140	1	$\bar{4}21$	42.19
2.125	2	510	42.51
2.114	35	420	42.74
2.101	40	$\bar{1}13$	43.01
2.025	30	$\bar{5}12$,$\bar{1}31$	44.71
2.020	30	$\bar{3}13$	44.83
1.982	9	222	45.74
1.966	30	131	46.13
1.959	5	$\bar{4}22$	46.31
1.922	6	113	47.25
1.900	2	421	47.84
1.8816	20	511	48.33
1.8765	18	600	48.47
1.8522	13	$\bar{6}02$	49.15
1.7481	2	$\bar{5}13$	52.29
1.7236	2	331	53.09
1.7096	1	$\bar{3}32$	53.56
1.6866	2	$\bar{4}23$	54.35
1.6640	7	$\bar{6}21$	55.15
1.6253	8	422	56.58
1.6190	7	620	56.82
1.6151	6	$\bar{7}11$	56.97
1.6066	6	$\bar{1}14$	57.30
1.6020	6	223,040	57.48
1.5979	10	$\bar{3}14$,512	57.64
1.5740	6	$\bar{7}12$,$\bar{5}31$	58.60
1.5599	3	710	59.18
1.5401	8	$\bar{1}33$,240	60.02
1.5240	7	332,$\bar{2}41$	60.72
1.5072	4	$\bar{3}33$	61.47

d (Å)	I	hkl	2θ (°)
1.4833	6	$\bar{2}24$	62.57
1.4765	4	$\bar{5}14$	62.89
1.4651	8	133	63.44
1.4609	6	602	63.64
1.4554	4	$\bar{7}13$	63.91
1.4507	6	204	64.14
1.4401	5	024	64.67
1.4342	6	042,711	64.97
1.4309	10	$\bar{2}42$	65.14
1.4270	5	$\bar{6}04$	65.34
1.4073	5	800	66.37
1.3916	7	440	67.22
1.3836	9	$\bar{5}33$	67.66
1.3502	8	$\bar{5}13$	69.57
1.3443	4	$\bar{4}42$	69.92
1.3289	8	622	70.85
1.3252	5	441	71.08
1.3208	9	333	71.35
1.3149	5	$\bar{7}31$	71.72
1.3127	3	$\bar{8}22$	71.86
1.3034	6	$\bar{7}14,\bar{6}24$	72.45
1.2948	3	$\bar{1}15$	73.01
1.2886	3	820	73.42
1.2726	4	150	74.50
1.2691	5	$\bar{9}11$	74.74
1.2558	4	$\bar{1}51$	75.67
1.2523	5	$\bar{5}15$	75.92
1.2488	5	134,$\bar{8}23$	76.17
1.2416	3	151	76.69
1.2280	2	910	77.70
1.2244	2	$\bar{7}33$	77.97
1.2208	6	442	78.24
1.2112	8	731,$\bar{6}42$	78.98

Strontium chloride hydroxide phosphate, $Sr_5Cl_{.65}(OH)_{.35}(PO_4)_3$

Sample

The sample was prepared by adding a Na_3PO_4 solution to a saturated solution of $SrCl_2$. After boiling, the precipitate was filtered, washed, dried, and heated to 1100 °C for one half hour. Analysis showed 3.07 percent chlorine.

Color

Colorless

Structure

Hexagonal, $P6_3/m$ (176), Z=2, isostructural with calcium hydroxyapatite, $Ca_5OH(PO_4)_3$; its structure was determined by Posner et al. [1958]. There is a complete solid solution between $Sr_5OH(PO_4)_3$ and $Sr_5Cl(PO_4)_3$. However, the structure of $Ca_5Cl(PO_4)_3$ was determined by Mackie et al. [1972] and found to be monoclinic, pseudohexagonal. The data here gave no indication of a departure from hexagonal.

NBS lattice constants:

a = 9.847(1)Å
c = 7.219(1)

Density

(calculated) 4.119 g/cm^3

Reference intensity

$I/I_{corundum}$ 3.0

Additional patterns

1. PDF 16-666 [General Electric Co. Ltd., Wembly England - for $Sr_5Cl(PO_4)_3$].

References

Mackie, P.E., Elliott, J.C., and Young, R.A.(1972) Acta Cryst. B28, 1840.

Posner, A.S., Perloff, A., and Diorio, A.F. (1958) Acta Cryst. 11, 308.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
8.51	2	100	10.39
5.50	2	101	16.10
4.93	3	110	17.98
4.263	13	200	20.82
4.070	9	111	21.82
3.609	13	002	24.65
3.325	11	102	26.79
3.225	20	210	27.64
2.942	95	211	30.36
2.910	100	112	30.70
2.842	55	300	31.45
2.755	3	202	32.47
2.645	1	301	33.86
2.464	1	220	36.44
2.404	2	212	37.37
2.365	9	310	38.02
2.247	2	311	40.10
2.232	6	302	40.37
2.162	9	113	41.75
2.132	2	400	42.35
2.096	2	203	43.12
2.033	35	222	44.52
1.978	11	312	45.83
1.956	4	329	46.39
1.928	25	213	47.10
1.888	15	321	48.16
1.861	15	410	48.90
1.835	14	402,303	49.63
1.804	9	004	50.54
1.721	<1	223, 322	53.18
1.695	1	114	54.07
1.687	2	313	54.32
1.662	1	204	55.22
1.655	4	412	55.49
1.640	1	330	56.02
1.6120	3	420	57.09
1.6004	2	331	57.54
1.5745	5	214	58.58
1.5417	3	502	59.95
1.5318	1	510	60.38
1.5236	10	304	60.74
1.5186	10	323	60.96
1.4975	7	511	61.91
1.4943	7	332	62.06
1.4725	1	413,422	63.08
1.4346	<1	314	64.95
1.4101	1	512	66.22
1.3775	2	404	68.00
1.3658	1	520	68.66
1.3563	1	333	69.21
1.3418	2	521	70.07
1.3389	3	423	70.24
1.3261	2	324	71.02
1.3224	3	602	71.25
1.3178	4	215	71.54
1.3067	2	432	72.24
1.2954	9	414	72.97
1.2774	7	522	74.17
1.2310	3	440	77.47
1.2142	1	334	78.75
1.2115	1	433	78.96
1.2021	3	424	79.70
1.1875	1	523	80.88
1.1680	4	514	82.52
1.1618	2	325	83.06
1.1543	2	532	83.72

Strontium oxide hydrate, $SrO_2 \cdot 8H_2O$

Sample
A solution of $SrCl_2$ was treated with a slight excess of three percent H_2O_2 and stirred. Dilute NH_4OH solution was added and the precipitate was dried at room temperature. Since the crystals were very thin platelets, orientation may have affected intensity measurements.

Color
Colorless

Structure
Tetragonal, P4/mcc (124), Z=2. The structure was determined by Vannerberg [1959].

NBS lattice constants:
a = 6.3432(5)Å
c =11.197(1)

Density
(calculated) 1.944 g/cm^3

Additional patterns
1. PDF card 12-521 [Vannerberg, 1959].
2. PDF card 2-1245 [Natta, 1932].

References

Natta, G. (1932). Gazz. Chim. Ital. 62, 444.
Vannerberg, N-G. (1959). Arkiv Kemi 14, 17.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.36	2	100	13.92
5.59	100	002	15.85
4.49	2	110	19.74
4.197	7	102	21.15
3.496	9	112	25.46
2.798	10	004	31.96
2.759	4	202	32.42
2.750	4	211	32.53
2.560	9	104	35.02
2.530	2	212	35.45
2.377	11	114	37.82
2.258	2	213	39.89
2.242	1	220	40.18
2.098	5	204	43.09
2.081	1	222	43.45
2.007	2	310	45.14
1.992	5	214	45.50
1.979	<1	302	45.81
1.889	2	312	48.14
1.866	1	006	48.75
1.791	8	106	50.95
1.758	1	320,215	51.97
1.723	1	116	53.10
1.687	<1	304	54.32
1.678	<1	322	54.64
1.608	<1	206	57.23
1.559	4	216	59.20
1.526	<1	402	60.64
1.490	<1	324	62.24
1.444	<1	332	64.48
1.434	<1	226	64.94
1.418	<1	420	65.81
1.399	4	008,306	66.79
1.394	1	217	67.11
1.379	1	404	67.90
1.374	1	422	68.18
1.367	4	108,316	68.62
1.348	<1	414	69.67
1.336	<1	118	70.41
1.319	<1	334	71.47
1.280	<1	208,326	73.98
1.255	1	218	75.71
1.187	1	228,416	80.93
1.167	1	308,336	82.59
1.155	<1	434	83.63
1.153	<1	522	83.85
1.148	1	318	84.30
1.139	<1	219	85.09
1.120	<1	0·0·10	86.91
1.103	1	1·0·10	88.61
1.095	1	328	89.41
1.086	<1	1·1·10	90.33
1.056	<1	2·0·10	93.67
1.0414	1	2·1·10	95.40
1.0352	1	418,516	96.16
1.0014	<1	2·2·10	100.56
.9960	1	428,526	101.31
.9891	<1	604	102.30
.9774	<1	3·1·10,614	104.01
.9754	<1	542	104.31
.9580	<1	2·1·11	107.04
.9446	<1	3·2·10	109.27
.9398	<1	438,536	110.10
.9231	<1	1·0·12	113.12
.9133	<1	1·1·12	115.00
.9053	<1	4·1·10	116.60
.9012	<1	528	117.44
.8952	<1	2·0·12	118.73
.8862	<1	2·1·12	120.72

Strontium phosphate, alpha $Sr_2P_2O_7$

Sample

The sample was prepared by adding dilute NH_4OH to a hot concentrated agueous solution of $SrCl_2$ and Na_3PO_4. The precipitate was filtered, washed with alcohol, and heated to 1200 °C for ten minutes.

Major impurities

∿ .05% Al, Ba, Ca, Mg, Co, and V.

Color

Colorless

Structure

Orthorhombic, Z=4, isostructural with α-$Ca_2P_2O_7$ [Wanmaker and ter Vrugt, 1967], [Ranby et al. 1955].

NBS lattice constants:

a = 8.917(2)Å
b = 13.169(2)
c = 5.400(1)

Density

(calculated) 3.657 g/cm^3

Reference intensity

$I/I_{corundum}$ = 2.3

Polymorphism

The alpha form is stable above 750 °C [Ranby et al., 1955]. Below 750 °C the alpha form very slowly changes to the beta form. The beta form is represented by PDF card 13-194 [Hoffman and Mooney, 1960].

Additional patterns

1. PDF card 12-362 [Ropp et al., 1959]

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
7.40	35	110	11.95
6.60	13	020	13.41
5.30	3	120	16.70
5.01	3	011	17.70
4.462	11	200	19.88
3.940	9	130	22.55
3.694	4	220	24.07
3.439	85	201	25.89
3.406	100	031	26.14
3.327	35	211	26.77
3.291	4	040	27.07
3.182	15	131	28.02
3.128	25	230	28.51
3.087	2	140	28.90
3.048	7	221	29.28
2.900	20	310	30.81
2.700	45	002	33.15
2.680	25	141	33.41
2.648	2	240,012	33.82
2.554	14	311	35.11
2.525	11	150	35.52
2.422	7	321	37.09
2.406	10	122	37.35
2.377	2	241	37.81
2.310	5	202	38.95
2.274	2	212	39.60
2.239	6	331	40.25
2.230	9	400	40.42
2.195	30	060	41.08
2.132	6	160	42.36
2.090	1	251	43.25
2.044	65	232	44.27
1.987	7	430	45.61
1.982	8	161	45.73
1.976	9	312	45.88
1.966	11	421	46.13
1.913	2	322	47.49
1.891	6	242	48.08
1.866	17	431	48.76
1.850	30	261	49.21
1.776	3	071	51.40
1.747	4	441	52.34
1.742	3	171	52.48
1.722	2	520	53.15
1.703	8	062,450	53.79
1.680	6	511	54.59
1.669	12	203	54.97
1.665	13	033	55.10
1.656	4	213	55.44
1.651	3	271	55.62

d (Å)	*I*	*hkl*	2θ(°)
1.6402	2	521	56.02
1.6370	3	133	56.14
1.6180	<1	223	56.86
1.6009	3	432	57.52
1.5903	7	370	57.94
1.5643	4	460	59.00
1.5554	3	143	59.37
1.5297	3	313	60.47
1.5249	2	371	60.68
1.5026	3	461	61.68

References

Hoffman, C.W.W.and Mooney, R.W.(1960). J. Electrochem. Soc. 107, 8541.

Ranby, P.W., Mash, D.H.,and Henderson, S.T.(1955). Brit. J. Appl. Phys. 6, Supplement 4 S18.

Ropp, R.C., Aia, M.A., Hoffman, C.W.W., Veleker, T.J., and Mooney, R.W. (1959). Anal. Chem. 31, 1163.

Wanmaker, W.L. and ter Vrugt, J.W. (1967). Philips Res. Rep. 22, 355.

Strontium phosphate, alpha $Sr_3(PO_4)_2$

Sample

The sample was prepared by heating a 3:2 molar mixture of $SrCO_3$ and $(NH_4)_2HPO_4$ at 700°C, grinding, and reheating at 1200 °C for 15 minutes.

Color

Colorless

Structure

Hexagonal, $R\bar{3}m$ (166), Z = 3, isostructural with $Ba_3(PO_4)_2$. The structure was determined by Zachariasen [1948].

NBS lattice constants:

a = 5.3871(2)Å
c = 19.780(1)

Density

(calculated) 4.537 g/cm^3

Reference intensity

$I/I_{corundum}$ 4.4

Polymorphism

α-$Sr_3(PO_4)_2$ undergoes a readily reversible, polymorphic inversion at 1305 °C to β-$Sr_3(PO_4)_2$ [Sarver et al., 1961].

Additional patterns

1. PDF card 14-271 [Sarver et al., 1961].
2. Zachariasen [1948].
3. PDF card 2-744 is for $Sr_5OH(PO_4)_3$ and not $Sr_3(PO_4)_2$.

References

Sarver, J. F., Hoffman, M. V., and Hummel, F. A. (1961). J. Electrochem. Soc. **108**, 1103.

Zachariasen, W. H. (1948). Acta Cryst. **1**, 263.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
6.60	1	003	13.40
4.554	7	101	19.52
4.225	1	012	21.01
3.393	10	104	26.24
3.016	100	015	29.59
2.694	85	110	33.23
2.494	<1	113	35.98
2.418	<1	107	37.15
2.318	3	021	38.82
2.271	11	202	39.66
2.198	11	009	41.03
2.186	2	018	41.27
2.110	14	024	42.82
2.087	7	116	43.32
2.009	35	205	45.08
1.821	20	1·0·10	50.05
1.799	2	027	50.69
1.7565	2	211	52.02
1.7360	<1	122	52.68
1.7031	9	119	53.78
1.6607	1	214	55.27
1.6107	20	125	57.14
1.5547	12	300	59.40
1.5087	6	0·2·10	61.40
1.4960	1	217	61.98
1.4360	<1	128	64.88
1.4243	<1	2·0·11	65.48
1.4066	1	306,1·1·12	66.41
1.3521	3	0·1·14	69.46
1.3468	10	220	69.77
1.3162	12	2·1·10	71.64
1.2913	<1	131	73.24
1.2827	<1	312	73.81
1.2746	<1	0·2·13	74.36
1.2697	2	309	74.70
1.2517	1	134	75.96
1.2298	7	315	77.56
1.2087	1	2·0·14	79.18
1.1844	8	1·1·15	81.14
1.1643	<1	401	82.84
1.1583	<1	042	83.37
1.1484	3	229	84.25
1.1353	<1	404	85.45
1.1288	<1	0·1·17	86.06
1.1188	3	045	87.02
1.1026	2	1·2·14	88.63
1.0828	4	1·3·10	90.69
1.0461	<1	324	94.84
1.0333	5	235	96.40
1.0182	4	410	98.32

d (Å)	*I*	*hkl*	2θ(°)
1.0161	3	1·0·19	98.59
1.0057	4	3·0·15	99.98
1.0049	2	4·0·10	100.09
0.9822	<1	238	103.30
.9784	<1	0·4·11	103.86
.9728	<1	416	104.71
.9711	<1	1·2·17	104.97
.9675	1	0·1·20	105.53
.9542	1	3·1·14	107.66
.9508	1	0·2·19	108.22
.9422	3	2·2·15	109.68
.9414	3	3·2·10	109.82
.9237	1	419	113.00
.9170	<1	054	114.29
.9105	<1	2·0·20	115.55
.9081	1	505	116.04
.8994	1	0·4·14	117.83
.8978	1	330	118.18
.8964	2	2·1·19	118.47
.8891	<1	1·1·21	120.07
.8828	<1	1·0·22	121.50
.8782	<1	422	122.59
.8680	<1	244	125.11
.8661	<1	336,4·1·12	125.59
.8626	2	1·2·20	126.51
.8605	4	425	127.05
.8531	1	2·3·14	129.08
.8438	1	0·5·10	131.80

Sucrose, $C_{12}H_{22}O_{11}$

Sample

The sample used was an NBS Standard Reference Material (Number 17)

moisture..... less than 0.01%
ash..... less than 0.01%
reducing substances... less than 0.02%

Color

Colorless

Optical data

Biaxial(-), N_α=1.540, N_β=1.558, N_γ=1.564; 2V is medium

Structure

Monoclinic, $P2_1$ (4), Z=2, structure determined by Beevers et al. [1952], and refined by Brown and Levy [1963].

NBS lattice constants:

a = 10.868(2)Å
b = 8.710(1)
c = 7.761(1)
β = 102.97(1)°

Density

(calculated) 1.588 g/cm^3

Reference intensity

$I/I_{corundum}$ = 0.7

Additional patterns

1. PDF card 6-0142 [Palmer, Agriculture Res. Service, Albany, California]

References

Brown, G.M. and Levy, H.A. (1963). Science **141**, 921.

Beevers, C.A., McDonald, T.R.R., Robertson, J.H., and Stern, F. (1952). Acta Cryst. **5**, 689.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
10.59	14	100	8.34
7.58	65	001	11.67
6.94	40	$\bar{1}01$	12.74
6.73	55	110	13.14
5.712	30	011	15.50
5.424	11	$\bar{1}11$	16.33
5.298	14	200	16.72
4.884	12	$\bar{2}01$	18.15
4.706	100	111	18.84
4.523	80	210	19.61
4.354	25	020	20.38
4.259	30	$\bar{2}11$	20.84
4.028	30	120	22.05
3.943	11	201	22.53
3.776	18	002,021	23.54
3.690	8	$\bar{1}21$	24.10
3.591	100	211	24.77
3.531	45	300	25.20
3.467	3	012,$\bar{2}02$	25.67
3.437	5	121	25.90
3.364	11	220	26.47
3.272	5	310	27.23
3.254	10	$\bar{2}21$	27.39
3.222	7	$\bar{2}12$	27.66
3.112	9	112	28.66
2.956	2	301	30.21
2.923	6	221	30.56
2.882	25	$\bar{1}22$	31.00
2.856	6	022	31.29
2.799	20	130,311+	31.95
2.777	4	$\bar{3}12$	32.21
2.742	10	320	32.63
2.711	4	$\bar{2}22$,031	33.01
2.677	10	$\bar{1}31$	33.44
2.661	4	212	33.65
2.648	2	400,122	33.82
2.586	5	$\bar{1}03$	34.66
2.574	4	131,$\bar{4}11$	34.82
2.545	3	230	35.24
2.521	5	003	35.58
2.504	6	$\bar{2}03$	35.83
2.496	7	$\bar{2}31$	35.95
2.479	9	$\bar{1}13$	36.20
2.444	5	321	36.74
2.430	6	$\bar{3}22$	36.96
2.406	9	$\bar{2}13$	37.34
2.349	40	222,$\bar{4}12$	38.28
2.339	16	401,231+	38.46
2.312	7	$\bar{3}03$	38.92
2.291	4	$\bar{4}21$	39.30

d (Å)	I	hkl	2θ(°)
2.258	14	113	39.89
2.253	11	$\bar{3}12$	39.98
2.234	10	$\bar{3}13$	40.33
2.189	5	$\bar{1}32$	41.20
2.171	5	$\bar{2}23,\bar{5}01$	41.57
2.133	1	140	42.34
2.101	2	203	43.02
2.091	2	$\bar{0}41$	43.23
2.075	7	$\bar{1}41,\bar{4}03$	43.58
2.060	6	123,510	43.92
2.042	10	213,$\bar{3}23$	44.33
2.028	4	141	44.64
2.014	1	240,232	44.97
2.000	1	$\bar{5}12$	45.30
1.971	1	402	46.00
1.956	4	$\bar{4}30$	46.39
1.942	3	$\bar{5}21$	46.74
1.929	5	$\bar{1}33,501$	47.07
1.924	5	$\bar{2}04,412$	47.21
1.904	6	520,033	47.72
1.895	4	$\bar{2}33,\bar{1}42$	47.96
1.887	4	042	48.18
1.885	3	$\bar{5}11$	48.23
1.870	2	$\bar{4}32$	48.66
1.855	3	340	49.08
1.823	3	142,313+	50.00
1.818	1	$\bar{3}32$	50.13
1.809	3	$\bar{3}33,\bar{3}14$	50.41
1.795	5	$\bar{4}22$	50.81
1.773	<1	$\bar{6}11$	51.50
1.764	2	600,521	51.79
1.753	2	$\bar{3}41$	52.12
1.733	2	024,$\bar{4}04$	52.79
1.718	1	150,242	53.27
1.698	4	051	53.97
1.693	5	$\bar{4}41,502$+	54.13
1.672	2	$\bar{6}21$	54.87
1.658	2	124	55.37
1.638	3	214	56.12
1.635	2	620	56.21

Zinc ammine bromide, $Zn(NH_3)_2Br_2$

Sample

The sample was made by dissolving Zn in hydrobromic acid and adding NH_4Br and NH_4OH.

Color

Colorless

Optical data

Biaxial (-), $N_\alpha = 1.650$, $N_\gamma = 1.712$

Structure

Orthorhombic, Imam (74), Z=4. The structure was determined by MacGillavry and Bijvoet [1936].

NBS lattice constants:

a = 8.419(1)
b = 8.816(1)
c = 8.122(1)

Density (calculated) 2.856 g/cm^3

Reference intensity

$I/I_{corundum} = 2.0$

References

MacGillavry, C. H. and Bijvoet, J. M. (1936). Z. Krist. **94**, 249.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.08	30	110	14.55
5.973	35	011	14.82
4.410	55	020	20.12
4.209	13	200	21.09
4.062	95	002	21.86
3.521	25	121	25.27
3.441	19	211	25.82
3.377	19	112	26.37
3.044	50	220	29.32
2.986	100	022	29.90
2.922	13	202	30.57
2.773	3	130	32.26
2.764	4	031	32.36
2.436	20	222	36.87
2.309	11	231	38.97
2.292	6	132	39.28
2.272	5	321	39.63
2.225	7	123	40.50
2.205	7	213,040	40.89
2.105	7	400	42.93
2.062	2	141	43.87
2.030	16	004,330	44.59
1.986	1	411	45.65
1.953	10	240	46.46
1.937	2	042	46.87
1.926	3	114	47.14
1.899	3	420	47.85
1.869	5	402	48.69
1.844	6	024	49.37
1.829	2	204	49.82
1.815	4	332	50.20
1.799	6	233	50.69
1.782	3	323	51.23
1.759	19	242	51.93
1.722	10	051	53.13
1.689	8	224	54.26
1.674	1	431,143	54.78
1.596	2	251	57.72
1.5320	2	512	60.37
1.4994	3	125	61.80
1.4936	4	251,044,+	62.09
1.4774	5	053	62.85
1.4611	2	053,404	63.63
1.4356	1	334	64.90
1.4256	2	442,161	65.41
1.4075	5	244	66.36
1.3870	2	424,260	67.47
1.3821	3	062	67.74
1.3534	2	006	69.38

Zinc fluoride hydrate, $ZnF_2 \cdot 4H_2O$

Sample
The sample was prepared by slow evaporation, at room temperature, of an aqueous solution of ZnF_2.

Color
Colorless

Optical data
Biaxial (-), N_α=1.460, N_β=1.458, N_γ=1.448; 2V is medium.

Structure
Orthorhombic, $P2_1ab$ (29), Z=4, isostructural with $NiF_2 \cdot 4H_2O$ [Rao et al., 1965].

NBS lattice constants:
a = 7.544(2)Å
b = 12.641(2)
c = 5.292(1)

Density
(calculated) 2.309 g/cm^3

Reference intensity
$I/I_{corundum} = 2.3$

Polymorphism
Easwaran and Srinivasan [1965] found by comparison of powder patterns that $ZnF_2 \cdot 4H_2O$ was isostructural with $FeF_2 \cdot 4H_2O$. However, Penfold and Taylor [1960] reported $FeF_2 \cdot 4H_2O$ as rhombohedral. This suggests a second form of $ZnF_2 \cdot 4H_2O$ exists.

References

Easwaran, K.R.K. and Srinivasan, R. (1965). Proc. Nuclear Physics - Solid State Physics Symposium, Calcutta, Part A, 171.

Penfold, B.R. and Taylor, M.R. (1960). Acta Cryst. **13**, 953.

Rao, K.V.K., Naidu, S.V.N., and Rao, P.V. (1965). Indian J. Pure Applied Phys. **3**, 68.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.29	6	001	16.73
4.87	100	011	18.19
4.844	100	120	18.30
4.098	70	111	21.67
3.776	7	200	23.54
3.577	5	121	24.87
3.297	6	031	27.02
3.160	25	040	28.22
3.072	4	201	29.04
3.023	9	131	29.52
2.985	40	211	29.91
2.762	20	221	32.39
2.592	10	012	34.58
2.555	12	141	35.10
2.484	3	231	36.13
2.449	6	112	36.67
2.323	10	122	38.73
2.281	4	051	39.47
2.236	14	311	40.30
2.202	3	241	40.96
2.184	14	151	41.31
2.167	16	202	41.65
2.148	3	132	42.02
2.135	4	212	42.29
2.029	16	160,042	44.62
1.999	4	331	45.32
1.957	4	061	46.35
1.952	8	251	46.49
1.927	4	232	47.13
1.887	8	400	48.19
1.845	2	341	49.36
1.804	6	312	50.54
1.786	12	242	51.09
1.759	13	411	51.94
1.751	18	322	52.20
1.738	8	261	52.63
1.709	4	071	53.59
1.689	2	351	54.25
1.673	2	332	54.84
1.667	4	171	55.06
1.658	4	123	55.36
1.644	4	252	55.88
1.619	3	440	56.83
1.615	5	360	56.97
1.610	5	162	57.18
1.589	2	133	57.96
1.581	2	080	58.32
1.579	2	342	58.41
1.557	2	271	59.29
1.544	1	361	59.85
1.541	3	043	60.02
1.537	1	402	60.19
1.4934	5	233	62.10
1.4671	5	520	63.34

Additional patterns
1. PDF card 1-253 [New Jersey Zinc Co.]

Structure

Orthorhombic, Pnnm (58), Z=2. The structure was determined by Döll and Klemm [1939], and refined by Brackett et al. [1963]. It is isostructural with $CaCl_2$ [van Bever and Nieuwenkamp, 1935].

Lattice parameters

a=6.584(6), b=6.871(6), C=4.342(4)Å [Brackett et al., 1963].

Density

(calculated) 3.380 g/cm^3

Thermal parameters

Isotropic, overall B=1.0

Scattering factors

Ca^{2+} [International Tables, 1962]
Br^- [Cromer and Waber, 1965]

Scale factor

(integrated intensities) 2.474×10^4

Additional patterns

1. PDF card 2-535 [Döll and Klemm, 1939]

Reference

van Bever, A.K.and Nieuwenkamp, W.(1935). Z.Krist. 90, 374.
Brackett, E.B.,Brackett, T.E.,and Sass, R.L.(1963) J. Inorg. Nucl. Chem. 25, 1295.
Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.
Döll, W. and Klemm, W. (1939). Z. anorg.u.allgem. Chem. 241, 233.
International Tables for X-ray Crystallography III (1962), 204.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	$2\theta(°)$ λ = 1.54056 Å
4.75	20	1 1 0	18.66
3.672	9	0 1 1	24.22
3.625	3	1 0 1	24.54
3.435	1	0 2 0	25.92
3.292	21	2 0 0	27.06
3.206	100	1 1 1	27.80
3.046	52	1 2 0	29.30
2.968	1	2 1 0	30.08
2.494	5	1 2 1	35.98
2.451	38	2 1 1	36.64
2.377	12	2 2 0	37.82
2.171	15	0 0 2	41.56
2.085	1	2 2 1	43.36
2.026	23	0 3 1	44.70
1.975	2	1 1 2	45.92
1.958	3	3 0 1	46.32
1.883	15	3 1 1	48.28
1.850	8	3 2 0	49.22
1.812	5	2 0 2	50.30
1.768	15	1 2 2	51.66
1.725	8	2 3 1	53.04
1.662	4	1 4 0	55.22
1.646	5	4 0 0	55.80
1.603	5	2 2 2	57.44
1.585	1	3 3 0	58.16
1.552	1	1 4 1	59.50
1.523	4	2 4 0	60.76
1.502	1	4 1 1	61.70
1.408	5	3 2 2	66.34
1.404	3	4 2 1	66.52
1.385	4	1 1 3	67.60
1.353	1	3 4 0	69.42
1.320	3	1 4 2	71.42
1.312	3	4 0 2	71.92
1.301	3	2 1 3	72.60
1.285	4	1 5 1	73.66
1.280	2	3 3 2	74.00
1.278	6	4 3 1	74.16
1.247	3	2 4 2	76.32
1.240	2	5 1 1	76.84
1.230	1	5 2 0	77.58
1.223	3	0 3 3	78.04
1.217	1	2 5 1	78.52
1.190	2	3 1 3	80.68
1.148	2	3 4 2	84.28
1.147	2	2 3 3	84.38
1.145	2	0 6 0	84.54
1.125	2	3 5 1	86.42
1.086	1	0 0 4	90.40
1.070	1	5 2 2	92.10

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.051	1	6 1 1	94.22
1.022	1	1 2 4	97.76
1.016	1	5 4 1	98.58
1.013	1	0 6 2	99.00
.985	2	1 5 3	102.84
.982	2	4 3 3	103.34
.968	1	2 6 2	105.44
.964	1	5 1 3 +	106.02
.942	1	5 4 2 +	109.76
.940	1	4 6 0	110.06
.936	1	3 2 4	110.74
.929	1	5 5 1	112.06
.919	2	2 7 1 +	113.84
.909	1	1 4 4	115.88
.907	1	3 5 3 +	116.20
.906	1	4 0 4	116.42
.884	1	2 4 4	121.24
.863	1	4 6 2	126.48
.854	1	1 1 5	128.76
.852	1	1 8 0	129.50
.851	1	6 4 2	129.74
.814	1	5 2 4	142.38
.812	1	0 3 5	143.12
.808	1	7 3 2	145.02
.802	1	3 1 5	147.68
.800	1	3 8 0	148.76
.795	1	5 5 3	151.56
.793	1	1 8 2	152.62
.789	2	2 7 3 +	155.20
.788	1	0 6 4	155.78
.787	1	8 2 1 +	156.52

Calculated Pattern *(Integrated)*			
d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
4.75	18	1 1 0	18.65
3.671	9	0 1 1	24.23
3.625	3	1 0 1	24.54
3.435	1	0 2 0	25.91
3.292	20	2 0 0	27.06
3.206	100	1 1 1	27.80
3.046	51	1 2 0	29.30
2.969	1	2 1 0	30.08
2.493	6	1 2 1	35.99
2.451	41	2 1 1	36.64
2.377	13	2 2 0	37.82
2.171	17	0 0 2	41.56
2.085	1	2 2 1	43.36
2.026	27	0 3 1	44.70
1.975	3	1 1 2	45.92
1.959	4	3 0 1	46.32
1.936	1	1 3 1	46.89
1.884	18	3 1 1	48.28
1.850	10	3 2 0	49.23
1.812	7	2 0 2	50.30
1.768	18	1 2 2	51.66
1.725	11	2 3 1	53.03
1.718	1	0 4 0	53.29
1.662	5	1 4 0	55.22
1.646	6	4 0 0	55.81
1.603	6	2 2 2	57.44
1.585	2	3 3 0	58.17
1.552	1	1 4 1	59.50
1.523	5	2 4 0	60.77
1.502	1	4 1 1	61.71
1.408	7	3 2 2	66.34
1.405	1	4 2 1	66.51
1.385	6	1 1 3	67.60
1.353	2	3 4 0	69.42
1.347	1	0 4 2	69.75
1.320	4	1 4 2	71.42
1.312	5	4 0 2	71.93
1.301	4	2 1 3	72.61
1.285	6	1 5 1	73.66
1.280	1	3 3 2	74.00
1.277	9	4 3 1	74.17
1.247	5	2 4 2	76.32
1.239	3	5 1 1	76.85
1.230	2	5 2 0	77.58
1.224	4	0 3 3	78.04
1.217	1	2 5 1	78.51
1.190	3	3 1 3	80.68
1.183	1	5 2 1	81.25
1.148	2	3 4 2	84.28
1.147	2	2 3 3	84.39

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.145	2	0 6 0	84.54
1.125	4	3 5 1	86.43
1.111	1	5 1 2	87.78
1.086	1	0 0 4	90.41
1.082	1	2 6 0	90.82
1.070	2	5 2 2	92.10
1.051	2	6 1 1	94.22
1.045	1	5 4 0	94.96
1.031	1	2 0 4	96.70
1.022	3	1 2 4	97.76
1.016	1	5 4 1	98.60
1.013	2	0 6 2	99.01
.987	1	2 2 4	102.54
.985	3	1 5 3	102.84
.982	4	4 3 3	103.34
.968	1	2 6 2	105.44
.965	1	6 3 1	105.94
.964	2	5 1 3	106.02
.947	1	1 7 1	108.78
.942	1	6 2 2	109.74
.942	1	5 4 2	109.77
.940	2	4 6 0	110.05
.936	2	3 2 4	110.73
.929	2	5 5 1	112.07
.925	1	6 4 0	112.81
.919	3	2 7 1	113.83
.919	1	7 0 1	113.85
.911	1	7 1 1	115.43
.909	1	1 4 4	115.89
.907	2	3 5 3	116.18
.907	1	7 2 0	116.22
.906	2	4 0 4	116.43
.884	2	2 4 4	121.25
.878	1	3 7 1	122.75
.870	1	7 3 0	124.58
.867	1	6 1 3	125.25
.863	3	4 6 2	126.49
.854	2	1 1 5	128.76
.852	1	1 8 0	129.50
.851	2	6 4 2	129.75
.847	1	5 4 3	130.77
.847	1	3 4 4	130.97
.837	2	7 2 2	133.92
.833	2	2 1 5	135.09
.828	1	4 7 1	137.10
.823	1	8 0 0	138.76
.817	1	6 3 3	141.10
.814	2	5 2 4	142.37
.812	3	0 3 5	143.11
.808	2	7 3 2	145.02

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
.806	1	1 7 3	145.64
.802	3	3 1 5	147.68
.800	2	3 8 0	148.76
.798	1	6 5 2	149.96
.795	3	5 5 3	151.55
.793	4	1 8 2	152.60
.792	1	6 6 0	152.92
.789	5	2 7 3	155.18
.789	2	7 0 3	155.21
.788	3	2 3 5	155.41
.788	4	0 6 4	155.78
.787	2	8 2 1	156.27
.787	1	5 7 0	156.35
.784	3	7 1 3	158.90

Calcium chloride hydrate, $CaCl_2 \cdot 4H_2O$

Structure
Triclinic, $P\bar{1}$ (2), Z=2. The structure was determined by Thewalt and Bugg [1973].

Lattice parameters
a=6.593(2), b=6.364(5), c=8.557(3)Å, α=97.77(5), β=93.52(4), γ=110.56(3)° [ibid.]

Density
(calculated) 1.838 g/cm^3

Thermal parameters
Anisotropic [ibid.]

Polymorphism
Three crystalline forms have been described. [Gmelins Handbuch, 1957]. The form characterized here apparently corresponds to the α-form [Thewalt and Bugg, 1973]

Scattering factors
Ca^{2+}, Cl^- [Cromer and Waber,1965], corrected for dispersion using terms Δf' and Δf'' from Cromer and Liberman [1970].

Scale factor
(integrated intensities)0.2942 x 10^4

Additional patterns
1. PDF card 1-1080 [Hanawalt et al., 1938]

Reference

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Gmelins Handbuch der Anorganischen Chemie.Calcium, Teil B (1957). Pg. 468.

Hanawalt, J.D., Rinn, H.W., and Frevel, L.K.(1938) Ind. Eng. Chem. Anal. Ed. **10**, 457.

Thewalt, U. and Bugg, C.E. (1973). Acta Cryst.B29 615.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
6.13	51	1 0 0	14.44
5.87	91	0 1 0	15.08
5.31	29	-1 1 0	16.68
5.25	27	-1 0 1 +	16.88
4.70	28	1 0 1	18.86
4.60	100	1 -1 1	19.28
4.48	3	0 1 1	19.82
4.40	2	-1 1 1	20.18
3.729	9	0 -1 2	23.84
3.633	15	1 1 0	24.48
3.567	53	-1 -1 1	24.94
3.383	4	1 -1 2	26.32
3.295	38	1 0 2	27.04
3.243	4	-2 1 0	27.48
3.222	16	-1 1 2	27.66
3.180	22	0 1 2	28.04
3.129	34	-1 2 0	28.50
3.064	33	2 0 0	29.12
3.056	24	1 -2 1	29.20
3.021	6	-1 -1 2	29.54
2.996	38	2 -1 1 +	29.80
2.938	62	0 2 0	30.40
2.930	42	0 -2 1	30.48
2.826	31	-1 2 1	31.64
2.806	23	0 0 3	31.86
2.778	4	2 0 1	32.20
2.715	71	0 -1 3	32.96
2.667	9	1 -2 2	33.58
2.657	22	-2 2 0	33.70
2.629	74	-2 0 2 +	34.08
2.609	21	-2 1 2	34.34
2.572	19	2 -2 1	34.86
2.535	9	1 -1 3	35.38
2.498	14	-2 2 1	35.92
2.445	6	1 0 3	36.72
2.433	10	-1 1 3 +	36.92
2.398	29	-2 -1 1	37.48
2.382	65	0 1 3 +	37.74
2.350	18	2 0 2	38.26
2.300	17	2 -2 2	39.14
2.239	22	0 2 2	40.24
2.234	20	-2 -1 2	40.34
2.224	16	1 -2 3 +	40.52
2.219	30	-1 -2 2	40.62
2.205	62	2 1 1 +	40.90
2.198	60	-2 2 2	41.02
2.193	25	-3 1 0	41.12
2.156	30	-2 1 3 +	41.86
2.105	8	0 0 4 +	42.94
2.100	8	-1 3 0	43.04

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.096	8	0 -1 4	43.12
2.090	26	2 -1 3	43.26
2.066	16	-1 0 4 +	43.78
2.055	6	1 1 3	44.02
2.041	6	-3 0 1	44.34
2.004	30	2 -3 1 +	45.20
1.999	18	-3 1 2	45.34
1.994	6	1 -3 2	45.46
1.980	6	2 -2 3 +	45.80
1.974	13	-1 3 1 +	45.94
1.958	6	0 3 0 +	46.32
1.934	1	3 0 1	46.94
1.919	7	-2 3 1	47.32
1.901	6	0 -3 2	47.80
1.897	4	3 -1 2	47.92
1.883	2	0 1 4	48.28
1.878	3	0 2 3	48.42
1.865	1	0 -2 4	48.78
1.851	3	1 -2 4	49.18
1.843	3	-2 -2 1	49.42
1.838	2	-2 0 4	49.54
1.817	5	2 2 0	50.18
1.784	5	-2 -2 2 +	51.16
1.759	6	3 0 2	51.94
1.754	7	-2 3 2 +	52.10
1.750	16	0 -3 3	52.24
1.745	9	3 1 0	52.40
1.720	1	-1 -3 1	53.20
1.716	4	2 2 1	53.36
1.696	5	0 -1 5 +	54.04
1.691	8	2 -2 4 +	54.18
1.679	4	-1 -3 2	54.60
1.675	3	-1 0 5	54.76
1.672	2	0 3 2	54.88
1.664	5	-3 2 3 +	55.14
1.659	7	3 1 1	55.34
1.647	3	2 0 4	55.76
1.635	7	-4 1 0	56.20
1.631	4	-4 1 1	56.38
1.622	9	-4 2 0	56.70
1.608	6	1 3 1	57.26
1.603	4	-4 2 1	57.44
1.592	2	-3 -1 3 +	57.88
1.582	3	4 -1 1 +	58.26
1.578	5	1 0 5 +	58.42
1.572	4	2 2 2	58.70
1.567	3	3 0 3	58.88
1.564	3	-2 4 0	59.00
1.563	3	-1 4 0	59.06
1.560	3	-3 0 4	59.16
1.555	2	-2 0 5	59.38
1.551	2	0 1 5	59.54
1.541	3	1 -4 2	59.96
1.533	3	3 -3 3 +	60.34
1.514	1	-2 1 5	61.16
1.506	1	-2 4 1	61.52
1.498	5	-4 0 2	61.90
1.493	10	-2 -1 5 +	62.14
1.484	3	1 3 2 +	62.54
1.481	3	4 -3 1	62.70
1.474	3	3 -2 4 +	63.02
1.468	8	0 4 0	63.28
1.465	6	-3 3 3 +	63.44
1.454	1	-3 -1 4	63.98
1.452	1	-1 -3 4	64.06
1.446	2	-3 -2 2	64.40
1.442	3	1 2 4	64.58
1.436	1	1 1 5	64.88
1.431	2	-3 4 1 +	65.14
1.428	3	3 -4 2	65.28
1.424	3	-4 2 3	65.48
1.420	4	0 -1 6	65.70
1.417	3	-4 0 3 +	65.88
1.414	5	1 -3 5 +	66.04
1.407	4	-4 3 2 +	66.36
1.403	6	0 0 6 +	66.58
1.391	7	-2 2 5 +	67.24
1.377	2	-2 -3 3 +	68.00
1.367	4	4 -1 3 +	68.60
1.358	7	-2 -2 5 +	69.12
1.355	5	-3 4 2	69.30
1.344	3	-4 1 4 +	69.96
1.340	2	-1 1 6	70.16
1.334	1	2 -4 4	70.54
1.331	2	4 -3 3	70.74
1.327	2	0 3 4	70.96
1.323	3	1 4 0 +	71.20
1.317	1	-1 -3 5	71.56
1.314	1	-3 -1 5	71.80
1.311	1	-1 -2 6	71.98
1.305	3	-4 -1 3 +	72.36
1.302	2	-2 4 3 +	72.54
1.297	1	3 -1 5	72.88
1.286	1	-1 4 3	73.56
1.283	4	2 1 5	73.82
1.271	1	2 2 4	74.64
1.267	1	-5 3 0	74.90
1.255	1	1 -5 1	75.74
1.254	1	3 1 4	75.82

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.13	46	1 0 0	14.44
5.87	86	0 1 0	15.07
5.31	28	-1 1 0	16.67
5.26	16	-1 0 1	16.85
5.25	12	0 -1 1	16.88
4.70	28	1 0 1	18.86
4.60	100	1 -1 1	19.28
4.48	2	0 1 1	19.81
4.40	2	-1 1 1	20.18
3.731	10	0 -1 2	23.83
3.633	16	1 1 0	24.48
3.568	57	-1 -1 1	24.94
3.383	4	1 -1 2	26.32
3.295	42	1 0 2	27.04
3.244	4	-2 1 0	27.47
3.223	17	-1 1 2	27.66
3.179	25	0 1 2	28.05
3.143	4	1 1 1	28.37
3.129	37	-1 2 0	28.50
3.065	38	2 0 0	29.11
3.054	7	1 -2 1	29.22
3.021	5	-1 -1 2	29.54
2.995	6	-2 0 1	29.80
2.995	37	2 -1 1	29.80
2.937	74	0 2 0	30.41
2.930	2	0 -2 1	30.48
2.825	35	-1 2 1	31.64
2.807	24	0 0 3	31.86
2.777	4	2 0 1	32.20
2.716	84	0 -1 3	32.95
2.673	3	-1 0 3	33.49
2.667	6	1 -2 2	33.57
2.657	22	-2 2 0	33.70
2.639	2	0 2 1	33.94
2.629	81	-2 0 2	34.07
2.624	25	0 -2 2	34.14
2.610	20	-2 1 2	34.33
2.571	22	2 -2 1	34.86
2.535	10	1 -1 3	35.38
2.499	17	-2 2 1	35.91
2.446	7	1 0 3	36.72
2.434	1	-1 -1 3	36.89
2.432	11	-1 1 3	36.93
2.397	34	-2 -1 1	37.49
2.385	2	2 1 0	37.68
2.382	73	0 1 3	37.74
2.380	7	-1 2 2	37.78
2.350	21	2 0 2	38.26
2.338	1	1 2 0	38.47
2.300	20	2 -2 2	39.14
2.239	25	0 2 2	40.24
2.234	18	-2 -1 2	40.35
2.225	10	1 -2 3	40.51
2.224	2	0 -2 3	40.53
2.219	29	-1 -2 2	40.63
2.204	64	2 1 1	40.90
2.203	18	-2 0 3	40.94
2.198	32	-2 2 2	41.03
2.193	5	-3 1 0	41.12
2.156	21	-2 1 3	41.86
2.156	3	1 2 1	41.86
2.156	14	-3 1 1	41.87
2.107	1	1 -3 1	42.88
2.105	9	0 0 4	42.93
2.100	3	-1 3 0	43.05
2.096	5	0 -1 4	43.11
2.090	32	2 -1 3	43.25
2.067	14	-1 0 4	43.76
2.066	8	-3 2 0	43.78
2.055	7	1 1 3	44.02
2.041	6	-3 0 1	44.33
2.006	4	3 -2 1	45.16
2.004	37	2 -3 1	45.21
1.998	3	-3 1 2	45.36
1.993	3	1 -3 2	45.47
1.980	5	2 -2 3	45.79
1.978	1	-1 -2 3	45.83
1.976	5	-1 -1 4	45.89
1.973	12	-1 3 1	45.95
1.959	3	2 0 3	46.32
1.958	5	0 3 0	46.33
1.934	2	3 0 1	46.93
1.919	9	-2 3 1	47.32
1.902	7	0 -3 2	47.79
1.896	1	3 -1 2	47.93
1.884	2	0 1 4	48.27
1.878	3	0 2 3	48.43
1.866	1	0 -2 4	48.78
1.851	4	1 -2 4	49.17
1.843	3	-2 -2 1	49.42
1.839	1	-2 0 4	49.53
1.816	8	2 2 0	50.18
1.784	7	-2 -2 2	51.16
1.782	1	-1 3 2	51.22
1.759	7	3 0 2	51.94
1.754	5	-2 3 2	52.10
1.753	1	-3 0 3	52.14
1.749	20	0 -3 3	52.24
1.743	2	3 1 0	52.44
1.722	1	-1 -3 1	53.14

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.715	5	2 2 1	53.37
1.698	2	1 1 4	53.95
1.696	4	0 -1 5	54.03
1.695	2	1 3 0	54.05
1.692	8	2 -2 4	54.17
1.689	1	2 1 3	54.25
1.679	5	-1 -3 2	54.61
1.675	1	-1 0 5	54.76
1.671	1	0 3 2	54.88
1.664	5	-3 2 3	55.14
1.663	1	3 -2 3	55.17
1.663	3	3 -3 2	55.19
1.659	8	3 1 1	55.35
1.647	3	2 0 4	55.76
1.635	10	-4 1 0	56.20
1.629	1	-4 1 1	56.43
1.622	14	-4 2 0	56.71
1.607	8	1 3 1	57.26
1.602	1	-4 2 1	57.48
1.592	3	-3 -1 3	57.88
1.589	1	0 2 4	57.98
1.583	1	-1 1 5	58.25
1.582	2	4 -1 1	58.27
1.580	2	0 -2 5	58.37
1.579	2	1 -4 1	58.39
1.577	2	1 0 5	58.47
1.572	4	2 2 2	58.70
1.567	1	3 0 3	58.90
1.564	3	-2 4 0	58.99
1.563	1	-1 4 0	59.07
1.561	2	-3 0 4	59.15
1.555	2	-2 0 5	59.39
1.551	1	0 1 5	59.54
1.542	4	1 -4 2	59.96
1.533	2	3 -3 3	60.32
1.533	2	4 0 0	60.34
1.514	1	-2 1 5	61.15
1.506	1	-2 4 1	61.51
1.498	4	-4 0 2	61.90
1.498	2	4 -2 2	61.90
1.493	7	0 3 3	62.13
1.492	8	-2 -1 5	62.15
1.485	1	4 -1 2	62.47
1.484	4	1 3 2	62.55
1.480	2	4 -3 1	62.70
1.478	1	4 0 1	62.84
1.476	1	2 -1 5	62.93
1.474	2	3 -2 4	63.01
1.473	1	3 -1 4	63.07
1.469	12	0 4 0	63.27
1.465	2	-3 3 3	63.42
1.464	1	-4 1 3	63.50
1.454	1	-3 -1 4	63.98
1.452	1	-1 -3 4	64.06
1.446	2	-3 -2 2	64.40
1.442	4	1 2 4	64.59
1.436	1	1 1 5	64.89
1.431	1	2 3 0	65.14
1.431	2	-3 4 1	65.14
1.428	4	3 -4 2	65.28
1.424	3	-4 2 3	65.50
1.420	5	0 -1 6	65.71
1.417	1	2 2 3	65.86
1.417	1	-4 0 3	65.86
1.414	5	1 -3 5	66.04
1.413	3	-2 4 2	66.09
1.408	2	2 0 5	66.34
1.407	4	-4 3 2	66.38
1.403	7	0 0 6	66.58
1.401	1	0 -4 3	66.69
1.392	4	-1 3 4	67.17
1.391	9	-2 2 5	67.23
1.379	1	-3 1 5	67.94
1.377	3	-2 -3 3	68.00
1.367	6	4 -1 3	68.59
1.365	1	0 2 5	68.69
1.358	4	-4 -1 2	69.09
1.358	1	0 -2 6	69.12
1.358	5	-2 -2 5	69.13
1.358	3	2 -3 5	69.13
1.355	2	-3 4 2	69.26
1.344	1	-1 -4 1	69.93
1.343	4	-4 1 4	69.97
1.340	2	-1 1 6	70.15
1.334	1	2 -4 4	70.55
1.331	2	4 -3 3	70.74
1.327	2	0 3 4	70.97
1.323	2	1 4 0	71.19
1.323	1	-3 3 4	71.20
1.317	1	-1 -3 5	71.56
1.314	1	-3 -1 5	71.80
1.311	1	-1 -2 6	71.98
1.305	2	-4 2 4	72.36
1.305	2	-4 -1 3	72.37
1.303	1	-2 1 6	72.48
1.302	1	-2 4 3	72.53
1.300	1	-5 1 1	72.65
1.297	1	3 -1 5	72.89
1.286	1	-1 4 3	73.56
1.283	5	2 1 5	73.82

Structure

Orthorhombic, Pnnm (58), Z=2 [Handy and Gregory, [1951]. The structure was determined independently and practically at the same time in four different laboratories and reported jointly in one paper [Tracy et al., 1961]

Lattice parameters

a=6.631, b=5.980, c=3.487Å [Tracy et al., 1961]

Density (calculated)

2.952 g/cm^3

Thermal parameters

Anisotropic;β_{11}=0.0137, β_{22}=0.0119 for all atoms

Atomic positions

Cr in 2a: 0,0,0
Cl in 4g: x,y,0 with x=0.360, y=0.275

Scattering factors

Cr^{2+}, Cl^- [Berghuis et al., 1955]

Scale factor

(integrated intensities) 0.5267 x 10^4

Additional patterns

1. PDF card 6-0159 [Handy and Gregory, 1951].
2. Oswald [1961]

Reference

Berghuis, J., Haanapel, IJ. M., Potters, M., Loopstra, B. O., MacGillavry, C. H., and Veenendahl, A. L. (1955). Acta Cryst. **8**, 478.

Handy, L. L. and Gregory, N. W. (1951). J. Chem. Phys. **19**, 1314.

Oswald, H. R. (1961). Helv. Chim. Acta **44**, 1049.

Tracy, J.W., Gregory, N.W., Lingafelter, E.C.,Dunitz, J.D., Mez, H.-C., Rundle, R.E., Scheringer, C., Yakel, H.L.,Jr., and Wilkinson, M.K. (1961). Acta Cryst. **14**, 927.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	$2\theta(°)$ λ = 1.54056 Å
4.44	100	1 1 0	19.98
3.314	8	2 0 0	26.88
3.011	15	0 1 1	29.64
2.990	2	0 2 0	29.86
2.899	36	2 1 0	30.82
2.743	41	1 1 1	32.62
2.230	19	2 1 1	40.42
2.220	15	2 2 0	40.60
2.147	49	1 2 1	42.04
2.073	4	3 1 0	43.62
1.909	2	1 3 0	47.60
1.873	2	2 2 1	48.58
1.867	18	3 0 1	48.74
1.782	2	3 1 1	51.22
1.743	10	0 0 2	52.44
1.731	8	0 3 1	52.86
1.708	3	2 3 0	53.60
1.674	4	1 3 1	54.78
1.623	6	1 1 2	56.68
1.543	1	2 0 2	59.88
1.534	3	2 3 1	60.28
1.494	8	2 1 2 +	62.06
1.480	3	3 3 0	62.72
1.452	4	4 1 1	64.06
1.450	6	4 2 0	64.18
1.371	3	2 2 2	68.36
1.363	1	3 3 1 +	68.84
1.334	1	3 1 2	70.52
1.269	1	2 4 1	74.72
1.240	1	5 0 1	76.84
1.220	2	2 3 2	78.28
1.214	1	5 1 1	78.78
1.177	1	1 5 0	81.76
1.167	3	3 4 1	82.62
1.135	2	0 4 2	85.48
1.128	2	3 3 2	86.10
1.125	2	1 1 3	86.46
1.115	3	4 2 2	87.42
1.079	1	2 1 3	91.12
1.071	1	2 5 1	92.02
1.069	3	1 2 3	92.18
1.029	2	3 0 3	96.96
1.004	1	0 3 3	100.20
.976	1	1 5 2	104.30
.934	1	4 5 1	111.04
.933	1	6 0 2	111.24
.933	1	5 3 2	111.32
.874	1	7 2 1 +	123.56
.872	1	0 0 4	124.14
.855	1	1 1 4	128.44
.848	1	3 4 3	130.70
.845	1	6 3 2	131.34

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
4.44	100	1 1 0	19.98
3.315	9	2 0 0	26.87
3.012	18	0 1 1	29.63
2.990	1	0 2 0	29.86
2.900	43	2 1 0	30.81
2.743	48	1 1 1	32.62
2.726	2	1 2 0	32.83
2.230	23	2 1 1	40.42
2.220	15	2 2 0	40.60
2.147	62	1 2 1	42.04
2.073	5	3 1 0	43.62
1.909	2	1 3 0	47.60
1.873	2	2 2 1	48.57
1.867	24	3 0 1	48.74
1.782	3	3 1 1	51.22
1.743	14	0 0 2	52.44
1.731	11	0 3 1	52.86
1.708	5	2 3 0	53.60
1.674	6	1 3 1	54.78
1.623	10	1 1 2	56.67
1.543	2	2 0 2	59.89
1.534	4	2 3 1	60.28
1.495	4	0 4 0	62.03
1.494	9	2 1 2	62.06
1.480	4	3 3 0	62.71
1.452	5	4 1 1	64.06
1.450	7	4 2 0	64.19
1.371	5	2 2 2	68.35
1.363	1	2 4 0	68.83
1.363	1	3 3 1	68.85
1.334	2	3 1 2	70.52
1.295	1	5 1 0	73.02
1.287	1	1 3 2	73.50
1.269	1	2 4 1	74.72
1.240	2	5 0 1	76.84
1.220	3	2 3 2	78.29
1.214	2	5 1 1	78.78
1.177	2	1 5 0	81.75
1.167	5	3 4 1	82.61
1.135	3	0 4 2	85.49
1.128	3	3 3 2	86.10
1.124	2	1 1 3	86.48
1.115	6	4 2 2	87.42
1.079	2	2 1 3	91.12
1.074	1	2 4 2	91.68
1.071	1	2 5 1	92.01
1.069	6	1 2 3	92.18
1.053	1	5 3 1	94.07
1.039	1	5 1 2	95.64
1.029	3	3 0 3	96.96

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.004	2	0 3 3	100.20
.993	1	1 3 3	101.77
.976	2	1 5 2	104.30
.961	1	2 3 3	106.56
.954	1	5 4 1	107.65
.948	2	1 6 1	108.61
.945	1	2 5 2	109.14
.940	1	4 1 3	110.08
.934	2	4 5 1	111.04
.933	1	6 0 2	111.22
.933	1	5 3 2	111.33
.931	1	6 3 1	111.58
.922	1	6 1 2	113.27
.921	1	2 6 1	113.59
.884	1	2 4 3	121.15
.874	2	7 2 1	123.55
.874	1	5 0 3	123.58
.872	3	0 0 4	124.16
.865	2	5 1 3	125.89
.855	2	1 1 4	128.44
.854	1	4 6 0	128.79
.847	4	3 4 3	130.71
.845	1	6 3 2	131.35
.837	1	2 6 2	133.86
.835	4	2 1 4	134.64
.830	2	0 7 1	136.35
.827	1	1 5 3	137.30
.824	1	7 1 2	138.24
.811	3	2 2 4	143.34
.808	2	2 5 3	144.68
.804	1	3 1 4	146.89
.801	2	5 3 3	148.40
.797	2	3 7 0	150.33
.794	1	6 1 3	152.02
.793	1	1 3 4	152.52
.792	2	6 4 2	153.24

Structure

Cubic, $P\bar{4}3m$ (215), Z=4. The structure was determined by Bradley and Jones[1933]. It was refined first by Westman [1965] and later by Heidenstam, Johannson, and Westman [1968]. This is the same phase of the copper-aluminum system that was called δ-CuAl (or Cu_9Al_4) by Bradley and Jones [1933] and by Weibke [1934]; it was later called γ-Cu_9Al_4 by Westman [1965] because its structure is very similar to that of γ-brass.

Lattice parameters

a=8.7027(5)Å (published value: 8.7023(5)Å) [Heidenstam et al., 1968]

Density (calculated)

6.850 g/cm^3

Thermal parameters

Isotropic [Heidenstam et al., 1968]

Atomic positions

The parameter values used were those in table 5 [Heidenstam et al., 1968], with half the "octahedral" Cu atoms in positions 6f and the other half in positions 6g [Westman, 1965].

Scattering factors

Cu^0, Al^0 [Cromer and Waber, 1965]: all factors were corrected for dispersion [Cromer, 1965].

Scale factor

(integrated intensities) 63.01 × 10^4

Additional patterns

1. PDF card 2-1254 [Weibke, 1934]

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ λ = 1.54056 Å
8.699	3	1 0 0	10.16
6.154	1	1 1 0	14.38
3.8903	4	2 1 0	22.84
3.5533	8	2 1 1	25.04
2.9006	8	3 0 0 +	30.80
2.5116	2	2 2 2	35.72
2.3259	3	3 2 1	38.68
2.0509	100	3 3 0 +	44.12
1.8990	1	4 2 1	47.86
1.8553	4	3 3 2	49.06
1.7762	4	4 2 2	51.40
1.7066	1	5 1 0 +	53.66
1.6749	1	5 1 1 +	54.76
1.5150	1	5 2 2	61.12
1.4503	8	6 0 0 +	64.16
1.4116	2	6 1 1 +	66.14
1.2832	2	6 3 1	73.78
1.2562	3	4 4 4	75.64
1.2306	2	5 5 0 +	77.50
1.1844	12	6 3 3 +	81.14
1.1053	1	7 3 2	88.36
1.0712	5	7 4 1	91.96
1.0553	1	8 2 0 +	93.76
1.0256	2	6 6 0 +	97.36
.9173	2	9 3 0 +	114.22
.8791	3	8 5 3 +	122.38
.8617	1	10 1 1 +	126.74
.8374	1	10 2 2 +	133.80
.8151	4	7 7 4 +	141.82
.7944	2	10 4 2	151.66

References

Bradley, A.J., and Jones,P. (1934). J.Inst. Metals **51**, 131.

Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. **18**, 104.

Cromer, D.T. (1965). Acta Cryst. 18, 17.

v. Heidenstam, O., Johannson, A., and Westman, S. (1968). Acta Chem. Scand. **22**, 653.

Weibke, F. (1934). Z. anorg.u.allgem. Chem. **220**, 293.

Westman, S. (1965). Acta Chem. Scand. 19, 1411.

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
8.703	3	1 0 0	10.16
6.154	1	1 1 0	14.38
3.8920	5	2 1 0	22.83
3.5529	10	2 1 1	25.04
2.9009	6	3 0 0	30.80
2.9009	4	2 2 1	30.80
2.5123	4	2 2 2	35.71
2.3259	4	3 2 1	38.68
2.1107	1	3 2 2	42.81
2.0513	100	3 3 0	44.11
2.0513	53	4 1 1	44.11
1.9460	1	4 2 0	46.64
1.8991	1	4 2 1	47.86
1.8554	6	3 3 2	49.06
1.7764	6	4 2 2	51.39
1.7067	1	4 3 1	53.66
1.7067	1	5 1 0	53.66
1.6748	1	5 1 1	54.76
1.6748	1	3 3 3	54.76
1.6161	1	4 3 2	56.93
1.5150	1	5 2 2	61.12
1.4505	8	6 0 0	64.15
1.4505	6	4 4 2	64.15
1.4118	2	6 1 1	66.13
1.4118	1	5 3 2	66.13
1.2831	3	6 3 1	73.78
1.2561	6	4 4 4	75.65
1.2307	3	5 5 0	77.49
1.2307	1	5 4 3	77.49
1.2069	1	6 4 0	79.32
1.1843	11	7 2 1	81.15
1.1843	1	5 5 2	81.15
1.1843	14	6 3 3	81.15
1.1629	1	6 4 2	82.96
1.1052	2	7 3 2	88.36
1.0712	12	7 4 1	91.95
1.0554	1	8 2 0	93.75
1.0554	1	6 4 4	93.75
1.0256	1	8 2 2	97.36
1.0256	4	6 6 0	97.36
.9983	2	6 6 2	101.00
.9854	2	7 5 2	102.83
.9174	3	9 3 0	114.21
.9174	2	7 5 4	114.21
.8791	2	9 4 1	122.38
.8791	6	8 5 3	122.38
.8617	1	7 7 2	126.74
.8617	3	10 1 1	126.74
.8534	2	8 6 2	129.01
.8453	1	9 4 3	131.36
.8374	3	10 2 2	133.80
.8374	1	6 6 6	133.80
.8298	1	9 5 2	136.34
.8151	2	8 7 1	141.83
.8151	12	7 7 4	141.83
.8151	2	8 5 5	141.83
.8046	1	8 7 2	146.43
.8046	1	10 4 1	146.43
.8012	1	10 3 3	148.09
.8012	2	9 6 1	148.09
.7944	10	10 4 2	151.66
.7879	2	9 5 4	155.72
.7879	2	11 1 0	155.72

Structure

Cubic, $I\bar{4}3m$ (217), Z=4. The structure was determined by Bradley and Gregory [1931] and refined by Heidenstam et al., [1968].

Lattice parameters

a=9.5892(3)Å (published value: 9.5888(3)Å) [Heidenstam et al., 1968]

Density (calculated)

9.166 g/cm^3

Thermal parameters

Isotropic [Heidenstam et al., 1968]

Atomic positions

Cu(1) in 8c, Cu(2) in 8c. The 12(Cu,Cd) in 12e and 24(Cu,Cd) in 24g are in random arrangement in each site, in the ratio of 1 Cu to 8 Cd.

Scattering factors

Cu^0, Cd^0 [Cromer and Waber, 1965]. All factors were corrected for dispersion [Cromer, 1965].

Scale factor

(integrated intensities) 159.5 × 10^4

Reference

Bradley, A.J. and Gregory, C.H. (1931). Phil. Mag. 12, 143.

Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.

Cromer, D.T. (1965). Acta Cryst. 18, 17.

v. Heidenstam, O., Johansson, A., and Westman, S. (1968). Acta Chem. Scand. 22, 653.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.9140	1	2 1 1	22.70
3.0315	9	3 1 0	29.44
2.7676	9	2 2 2	32.32
2.5630	14	3 2 1	34.98
2.3976	1	4 0 0	37.48
2.2597	100	4 1 1 +	39.86
2.0448	12	3 3 2	44.26
1.9577	7	4 2 2	46.34
1.8805	3	5 1 0 +	48.36
1.6445	1	5 3 0 +	55.86
1.5984	3	4 4 2 +	57.62
1.5556	2	5 3 2 +	59.36
1.5163	1	6 2 0	61.06
1.4797	2	5 4 1	62.74
1.4455	1	6 2 2	64.40
1.4139	4	6 3 1	66.02
1.3839	4	4 4 4	67.64
1.3562	4	5 5 0 +	69.22
1.3048	10	7 2 1 +	72.36
1.2814	1	6 4 2	73.90
1.2177	2	7 3 2 +	78.48
1.1803	2	7 4 1	81.48
1.1629	1	8 2 0 +	82.96
1.1301	1	6 6 0 +	85.94
1.1000	1	6 6 2	88.90
1.0857	2	7 5 2	90.38
1.0107	1	8 5 1 +	99.30
.9687	2	8 5 3 +	105.34
.9228	1	10 2 2 +	113.18
.8981	1	7 7 4 +	118.12
.8543	3	10 5 1 +	128.76
.8284	1	11 3 2 +	136.82

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
3.9148	1	2 1 1	22.70
3.0324	15	3 1 0	29.43
2.7682	15	2 2 2	32.31
2.5628	24	3 2 1	34.98
2.3973	2	4 0 0	37.48
2.2602	88	3 3 0	39.85
2.2602	100	4 1 1	39.85
2.0444	23	3 3 2	44.27
1.9574	14	4 2 2	46.35
1.8806	4	5 1 0	48.36
1.8806	2	4 3 1	48.36
1.7507	1	5 2 1	52.20
1.6445	2	5 3 0	55.86
1.6445	1	4 3 3	55.86
1.5982	2	6 0 0	57.63
1.5982	5	4 4 2	57.63
1.5556	1	6 1 1	59.36
1.5556	3	5 3 2	59.36
1.5162	2	6 2 0	61.07
1.4797	5	5 4 1	62.74
1.4456	3	6 2 2	64.39
1.4138	9	6 3 1	66.02
1.3841	9	4 4 4	67.63
1.3561	1	5 4 3	69.22
1.3561	7	5 5 0	69.22
1.3049	18	7 2 1	72.35
1.3049	1	5 5 2	72.35
1.3049	7	6 3 3	72.35
1.2814	2	6 4 2	73.90
1.2178	3	6 5 1	78.47
1.2178	3	7 3 2	78.47
1.1987	1	8 0 0	79.98
1.1804	5	7 4 1	81.47
1.1629	2	8 2 0	82.97
1.1629	2	6 4 4	82.97
1.1461	2	6 5 3	84.45
1.1301	2	6 6 0	85.94
1.1301	2	8 2 2	85.94
1.1000	3	6 6 2	88.90
1.0858	5	7 5 2	90.38
1.0590	1	8 3 3	93.34
1.0340	1	9 2 1	96.31
1.0108	1	7 5 4	99.29
1.0108	1	8 5 1	99.29
.9891	1	9 3 2	102.30
.9787	1	8 4 4	103.82
.9687	2	9 4 1	105.35
.9687	5	8 5 3	105.35
.9495	1	10 1 1	108.44
.9314	2	9 5 0	111.59
.9227	4	10 2 2	113.19
.9227	1	6 6 6	113.19
.8981	2	8 7 1	118.11
.8981	3	7 7 4	118.11
.8981	1	8 5 5	118.11
.8682	2	9 5 4	125.06
.8543	2	11 2 1	128.76
.8543	5	9 6 3	128.76
.8543	6	10 5 1	128.76
.8476	2	8 8 0	130.68
.8410	1	9 7 0	132.66
.8346	1	10 4 4	134.71
.8284	2	11 3 2	136.83
.8284	1	7 7 6	136.83
.8223	1	10 6 0	139.03
.8223	1	8 6 6	139.03
.8163	1	8 7 5	141.34
.8163	1	11 4 1	141.34
.8047	2	9 6 5	146.36
.7991	2	8 8 4	149.13
.7936	1	9 7 4	152.15
.7936	1	11 5 0	152.15
.7936	1	12 1 1	152.15
.7936	1	11 4 3	152.15
.7829	2	11 5 2	159.35

Copper hydrogen phosphite hydrate, $CuHPO_3 \cdot 2H_2O$

Structure
Orthorhombic, $P2_12_12_1$ (19), Z=4. The structure was determined by Handlovic [1969].

Lattice parameters
a=6.71, b=9.00, c=7.40Å [ibid.]

Density
(calculated) 2.67 g/cm^3

Thermal parameters
Isotropic [Handlovic]

Scattering factors
Cu^0, O^0, P^0 [International Tables, 1962]

Scale factor
(integrated intensities) 4.158×10^4

Reference

Handlovic, M. (1969). Acta Cryst. **B25**, 227

International Tables for X-ray Crystallography III (1962). 202, 210.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(^\circ)$ $\lambda = 1.54056$ Å
5.38	22	1 1 0	16.46
4.97	100	1 0 1	17.84
4.50	3	0 2 0	19.72
4.35	10	1 1 1	20.40
3.84	16	0 2 1	23.12
3.74	63	1 2 0	23.80
3.70	10	0 0 2	24.04
3.422	21	0 1 2	26.02
3.336	13	1 2 1	26.70
3.241	7	1 0 2	27.50
2.893	10	2 1 1 +	30.88
2.857	2	0 2 2	31.28
2.779	7	0 3 1	32.18
2.690	9	2 2 0	33.28
2.629	8	1 2 2	34.08
2.569	4	1 3 1	34.90
2.528	38	2 2 1	35.48
2.485	2	2 0 2	36.12
2.395	5	2 1 2	37.52
2.379	1	0 1 3	37.78
2.331	1	0 3 2	38.60
2.316	9	1 0 3	38.86
2.250	4	0 4 0	40.04
2.242	5	1 1 3	40.18
2.237	4	2 3 0	40.28
2.170	3	3 1 0	41.58
2.163	7	0 2 3	41.72
2.152	3	0 4 1	41.94
2.141	4	3 0 1	42.18
2.134	5	1 4 0	42.32
2.059	4	1 2 3	43.94
2.050	7	1 4 1	44.14
2.003	6	3 2 0	45.24
1.940	2	2 1 3	46.78
1.933	2	3 2 1	46.96
1.914	3	3 0 2 +	47.46
1.905	2	0 3 3	47.70
1.869	1	2 4 0	48.68
1.848	5	1 4 2 +	49.26
1.833	4	1 3 3	49.70
1.818	3	2 2 3	50.14
1.812	5	2 4 1 +	50.32
1.793	1	3 3 0	50.88
1.783	1	1 0 4	51.18
1.762	4	3 2 2	51.86
1.750	4	1 1 4	52.24
1.745	2	3 3 1	52.40
1.711	1	0 2 4	53.52
1.693	2	1 5 1	54.14
1.678	5	4 0 0	54.66

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.668	6	2 4 2	55.00
1.663	4	0 4 3	55.18
1.658	6	1 2 4 +	55.38
1.649	1	4 1 0	55.68
1.630	1	3 1 3	56.42
1.620	3	2 0 4	56.78
1.614	3	1 4 3	57.02
1.594	2	2 1 4	57.78
1.586	1	3 4 0	58.10
1.573	2	1 5 2 +	58.62
1.555	1	3 2 3	59.40
1.551	3	3 4 1	59.56
1.537	1	4 2 1	60.14
1.528	1	4 0 2	60.56
1.506	1	4 1 2	61.52
1.490	2	2 4 3	62.28
1.458	2	3 4 2 +	63.78
1.454	2	0 5 3	63.98
1.450	2	3 3 3	64.16
1.447	2	4 2 2	64.34
1.436	3	1 6 1 +	64.88
1.425	3	2 3 4 +	65.42
1.408	1	3 1 4	66.34
1.398	1	1 4 4	66.88
1.390	2	0 6 2	67.30
1.369	2	2 6 0	68.46
1.361	1	4 3 2 +	68.92
1.359	2	3 2 4	69.06
1.345	1	4 4 0	69.88
1.339	1	2 1 5	70.24
1.334	1	2 5 3 +	70.52
1.325	2	4 2 3	71.06
1.322	1	4 4 1	71.26
1.320	2	5 0 1	71.38
1.315	1	2 4 4	71.74
1.306	1	5 1 1	72.26
1.302	1	1 3 5	72.54
1.297	2	2 2 5	72.88
1.286	1	5 2 0	73.60
1.284	2	2 6 2	73.70
1.281	1	0 6 3	73.90
1.267	2	5 2 1 +	74.88
1.259	2	1 6 3 +	75.44
1.228	1	3 6 1	77.66
1.216	1	1 4 5	78.62
1.141	1	3 3 5 +	84.88
1.112	1	0 8 1 +	87.68
1.074	1	5 2 1	91.68
1.070	1	4 6 2	92.04
1.063	1	1 8 2	92.90
1.006	1	1 5 6	99.96

Calculated Pattern *(Integrated)*			
d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
5.38	21	1 1 0	16.46
4.97	100	1 0 1	17.83
4.50	3	0 2 0	19.71
4.35	10	1 1 1	20.39
3.84	17	0 2 1	23.11
3.74	70	1 2 0	23.79
3.70	9	0 0 2	24.03
3.422	23	0 1 2	26.02
3.355	1	2 0 0	26.55
3.336	14	1 2 1	26.70
3.240	8	1 0 2	27.51
3.056	3	2 0 1	29.20
3.049	10	1 1 2	29.27
2.893	11	2 1 1	30.88
2.858	2	0 2 2	31.27
2.780	9	0 3 1	32.17
2.690	11	2 2 0	33.28
2.629	10	1 2 2	34.07
2.568	4	1 3 1	34.90
2.528	45	2 2 1	35.48
2.485	3	2 0 2	36.11
2.396	6	2 1 2	37.51
2.379	1	0 1 3	37.78
2.330	1	0 3 2	38.60
2.315	11	1 0 3	38.87
2.250	5	0 4 0	40.04
2.242	5	1 1 3	40.19
2.236	2	2 3 0	40.30
2.171	3	3 1 0	41.57
2.163	8	0 2 3	41.72
2.153	3	0 4 1	41.93
2.141	5	3 0 1	42.17
2.133	5	1 4 0	42.33
2.059	5	1 2 3	43.94
2.050	9	1 4 1	44.15
2.003	8	3 2 0	45.24
1.941	3	2 1 3	46.77
1.933	2	3 2 1	46.96
1.914	2	3 0 2	47.46
1.914	1	2 3 2	47.46
1.905	2	0 3 3	47.69
1.869	2	2 4 0	48.69
1.850	3	0 0 4	49.21
1.848	5	1 4 2	49.27
1.833	5	1 3 3	49.70
1.818	3	2 2 3	50.14
1.812	1	0 1 4	50.31
1.812	5	2 4 1	50.32
1.793	1	3 3 0	50.88
1.783	1	1 0 4	51.18

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.761	6	3 2 2	51.87
1.749	5	1 1 4	52.25
1.743	1	3 3 1	52.46
1.711	2	0 2 4	53.51
1.692	2	1 5 1	54.15
1.677	8	4 0 0	54.67
1.668	8	2 4 2	55.01
1.662	1	0 4 3	55.21
1.658	6	1 2 4	55.37
1.657	2	3 0 3	55.41
1.649	1	4 1 0	55.69
1.630	2	3 1 3	56.42
1.620	4	2 0 4	56.78
1.614	3	1 4 3	57.03
1.594	2	2 1 4	57.78
1.586	2	3 4 0	58.10
1.575	1	0 3 4	58.57
1.573	3	1 5 2	58.62
1.555	1	3 2 3	59.39
1.551	4	3 4 1	59.55
1.538	2	4 2 1	60.13
1.528	1	4 0 2	60.55
1.506	2	4 1 2	61.51
1.490	4	2 4 3	62.28
1.458	2	3 4 2	63.79
1.458	1	2 5 2	63.79
1.454	1	0 5 3	63.98
1.450	2	3 3 3	64.16
1.447	1	4 2 2	64.34
1.436	1	4 3 1	64.86
1.436	4	1 6 1	64.88
1.427	1	1 1 5	65.34
1.425	3	2 3 4	65.42
1.408	2	3 1 4	66.33
1.398	2	1 4 4	66.89
1.390	2	0 6 2	67.30
1.369	3	2 6 0	68.46
1.361	1	4 3 2	68.91
1.361	1	1 6 2	68.93
1.359	3	3 2 4	69.06
1.345	1	4 4 0	69.89
1.339	2	2 1 5	70.23
1.334	1	3 4 3	70.53
1.334	1	2 5 3	70.53
1.326	3	4 2 3	71.05
1.323	1	4 4 1	71.20
1.320	2	5 0 1	71.37
1.315	2	2 4 4	71.73
1.306	1	5 1 1	72.26
1.302	2	1 3 5	72.54

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.297	4	2 2 5	72.89
1.286	1	5 2 0	73.59
1.284	2	2 6 2	73.71
1.282	1	0 6 3	73.89
1.267	1	5 2 1	74.88
1.267	1	1 5 4	74.89
1.259	1	4 3 3	75.44
1.259	1	1 6 3	75.45
1.249	1	5 1 2	76.13
1.228	2	5 6 1	77.66
1.216	1	1 4 5	78.61
1.204	1	3 4 4	79.53
1.179	1	5 0 3	81.60
1.169	1	5 1 3	82.45
1.143	1	0 5 5	84.72
1.142	1	2 7 2	84.83
1.141	1	3 3 5	84.88
1.141	1	0 3 6	84.95
1.124	1	1 7 3	86.52
1.112	2	0 8 1	87.67
1.112	1	3 6 3	87.69
1.074	1	6 2 1	91.67
1.072	1	3 1 6	91.83
1.070	1	4 6 2	92.05
1.063	2	1 8 2	92.90
1.018	1	4 6 3	98.29
1.006	1	1 5 6	99.95
1.002	2	2 1 7	100.48
.991	1	5 6 1	102.00
.986	1	1 3 7	102.71
.979	1	2 8 3	103.77
.970	1	3 8 2	105.16
.967	1	6 4 2	105.66
.945	1	4 5 5	109.25
.944	1	5 3 5	109.42

L-Cysteine, $HSCH_2 \cdot CH(NH_2) \cdot COOH$

Structure

Monoclinic, $P2_1(4)$, Z=4. The structure was determined by Harding and Long [1968].

Lattice parameters

a=11.51(1), b=5.240(5), c=9.517(10)Å, β=109.13° [ibid.]

Density

(calculated) 1.484 g/cm^3

Thermal parameters

Isotropic:

		carbon (1)	1.26
		" (11)	1.26
sulfur (1)	B=3.81	nitrogen (1)	1.26
sulfur (2)	4.99	" (11)	1.74
carbon (3)	2.37	oxygen (1)	1.58
" (13)	2.21	" (11)	1.74
" (2)	1.58	" (2)	2.45
" (12)	1.42	" (12)	2.45
		hydrogen (all)	1.42

Scattering factors

C^0, H^0, N^0, $O^{-1/2}$, S^0. The sulfur factors were corrected for the real part of the dispersion. [International Tables, 1962].

Scale factor

(integrated intensities) 0.5947×10^4

Additional patterns

1. PDF card 13-722 [Eli Lilly Co., Indianapolis, Indiana.]

Reference

Harding, M.M. and Long, H.A. (1968). Acta Cryst. B24, 1096.

International Tables for X-ray Crystallography III (1962), 202, 214.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
10.88	42	1	0	0	8.12
8.98	4	0	0	1	9.84
8.40	1	-1	0	1	10.52
6.02	3	1	0	1	14.70
5.52	2	-2	0	1	16.04
5.43	11	2	0	0	16.30
4.72	86	1	1	0 +	18.78
4.53	100	0	1	1	19.60
4.49	92	0	0	2	19.74
4.45	34	-1	1	1	19.94
4.21	14	-2	0	2	21.10
3.96	14	1	1	1	22.46
3.82	4	-3	0	1	23.24
3.802	15	-2	1	1	23.38
3.773	29	2	1	0	23.56
3.745	41	1	0	2	23.74
3.625	44	3	0	0	24.54
3.515	54	-1	1	2	25.32
3.422	34	-3	0	2	26.02
3.411	51	0	1	2	26.10
3.281	20	-2	1	2	27.16
3.227	58	2	1	1	27.62
3.166	4	-1	0	3	28.16
3.087	15	-2	0	3 +	28.90
3.046	3	1	1	2	29.30
3.035	3	3	0	1	29.40
2.996	7	0	0	3	29.80
2.980	53	3	1	0	29.96
2.866	4	-3	1	2	31.18
2.805	1	-3	0	3	31.88
2.761	19	-4	0	2	32.40
2.719	50	4	0	0	32.92
2.712	41	-1	1	3	33.00
2.673	3	1	0	3	33.50
2.660	25	-2	1	3	33.66
2.626	7	3	1	1	34.12
2.620	11	0	2	0	34.20
2.612	11	2	1	2	34.30
2.605	6	0	1	3	34.40
2.547	9	1	2	0	35.20
2.516	4	0	2	1	35.66
2.502	3	-1	2	1	35.86
2.473	7	-3	1	3	36.30
2.456	14	3	0	2	36.56
2.443	8	-4	1	2	36.76
2.412	2	4	1	0	37.24
2.403	2	1	2	1	37.40
2.394	2	4	0	1	37.54
2.382	17	1	1	3	37.74
2.370	9	-2	0	4	37.94

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.360	6	2 2 0 +	38.10
2.293	2	-1 2 2 +	39.26
2.273	6	-3 0 4	39.62
2.248	11	0 0 4	40.08
2.221	15	-4 1 3 +	40.58
2.208	2	2 2 1	40.84
2.177	4	4 1 1	41.44
2.161	5	-3 2 1 +	41.76
2.155	3	-1 1 4	41.88
2.146	4	1 2 2	42.06
2.121	5	-5 0 3 +	42.58
2.104	2	-4 0 4	42.96
2.100	2	-5 1 1	43.04
2.085	6	-3 1 4 +	43.36
2.081	8	-3 2 2	43.46
2.066	1	0 1 4	43.78
2.048	1	4 0 2	44.18
2.019	1	-1 2 3	44.86
2.009	1	3 0 3	45.10
1.998	1	-2 2 3	45.36
1.983	4	3 2 1	45.72
1.977	13	2 2 2	45.86
1.972	9	5 0 1 +	45.98
1.967	3	-5 1 3	46.12
1.952	1	-4 1 4	46.48
1.937	1	-4 2 1	46.86
1.926	1	1 1 4	47.16
1.915	2	-3 2 3	47.44
1.907	7	4 1 2	47.64
1.901	7	-4 2 2	47.82
1.886	1	4 2 0	48.20
1.875	2	3 1 3 +	48.50
1.871	3	1 2 3 +	48.62
1.845	2	5 1 1	49.36
1.841	3	-6 0 3	49.48
1.798	4	0 0 5 +	50.72
1.794	4	-4 0 5	50.86
1.791	5	-5 1 4 +	50.94
1.787	3	-6 1 1	51.06
1.764	7	-3 1 5 +	51.78
1.760	5	-2 2 4	51.92
1.753	3	-1 2 4	52.12
1.749	2	4 0 3	52.26
1.737	5	-6 1 3	52.66
1.725	1	1 3 0 +	53.06
1.715	4	0 3 1 +	53.38
1.711	3	-6 0 4	53.50
1.706	3	0 2 4	53.68
1.701	2	0 1 5	53.84
1.678	1	1 3 1 +	54.66

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.673	3	5 2 0	54.82
1.663	4	2 3 0 +	55.18
1.628	2	0 3 2	56.48
1.613	3	-2 3 2 +	57.04
1.607	3	1 1 5 +	57.30
1.599	3	3 1 4	57.58
1.594	3	6 1 1	57.78
1.583	2	1 3 2	58.24
1.573	1	3 3 0 +	58.62
1.569	2	-7 1 2	58.82
1.557	1	-6 0 5	59.32
1.553	2	7 0 0 +	59.46
1.543	2	-4 0 6	59.88
1.541	2	-5 2 4 +	59.98
1.529	1	-1 3 3	60.48
1.525	1	-3 2 5	60.68
1.507	2	4 0 4	61.50
1.496	1	2 1 5	61.96
1.493	2	-4 3 1	62.14
1.490	3	6 2 0 +	62.24
1.483	2	0 2 5	62.60
1.475	1	5 1 3 +	62.96
1.458	1	6 1 2	63.80
1.453	2	5 2 2	64.02
1.419	1	1 2 5	65.76
1.406	1	-2 3 4	66.44
1.384	1	3 1 5	67.64
1.380	2	-7 2 1 +	67.88
1.376	1	-8 1 3	68.08
1.373	1	-7 2 3	68.26
1.339	1	-6 2 5 +	70.26
1.313	2	6 2 2	71.84
1.310	2	-2 1 7	72.02
1.297	1	7 1 2	72.84
1.294	1	-1 4 1	73.04
1.287	1	-2 3 5	73.54
1.275	1	-9 0 3	74.34
1.271	1	-8 1 5	74.58
1.261	1	-8 2 2	75.32
1.252	1	-4 3 5	75.96

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
10.87	38	1	0	0	8.12
8.99	4	0	0	1	9.83
8.41	1	-1	0	1	10.50
6.03	3	1	0	1	14.69
5.52	2	-2	0	1	16.04
5.44	11	2	0	0	16.29
4.74	42	-1	0	2	18.71
4.72	71	1	1	0	18.78
4.53	100	0	1	1	19.59
4.50	89	0	0	2	19.73
4.45	32	-1	1	1	19.94
4.21	15	-2	0	2	21.10
3.95	15	1	1	1	22.46
3.82	3	-3	0	1	23.24
3.801	15	-2	1	1	23.38
3.773	29	2	1	0	23.56
3.744	45	1	0	2	23.75
3.625	49	3	0	0	24.54
3.515	61	-1	1	2	25.32
3.423	31	-3	0	2	26.01
3.412	44	0	1	2	26.09
3.281	23	-2	1	2	27.16
3.227	67	2	1	1	27.62
3.168	5	-1	0	3	28.15
3.089	9	-3	1	1	28.88
3.087	10	-2	0	3	28.90
3.046	3	1	1	2	29.29
3.035	2	3	0	1	29.41
2.997	5	0	0	3	29.78
2.981	67	3	1	0	29.95
2.866	5	-3	1	2	31.19
2.805	1	-3	0	3	31.88
2.761	23	-4	0	2	32.40
2.719	59	4	0	0	32.92
2.711	17	-1	1	3	33.02
2.674	2	1	0	3	33.49
2.660	32	-2	1	3	33.67
2.626	6	3	1	1	34.11
2.620	9	0	2	0	34.20
2.612	9	2	1	2	34.30
2.602	3	0	1	3	34.44
2.547	11	1	2	0	35.21
2.515	5	0	2	1	35.66
2.502	4	-1	2	1	35.87
2.473	8	-3	1	3	36.30
2.456	17	3	0	2	36.56
2.443	9	-4	1	2	36.76
2.413	2	4	1	0	37.23
2.403	1	1	2	1	37.40
2.394	4	4	0	1	37.54
2.382	21	1	1	3	37.74
2.370	10	-2	0	4	37.94
2.360	3	2	2	0	38.10
2.360	3	-1	0	4	38.10
2.293	1	-1	2	2	39.26
2.293	1	-5	0	1	39.27
2.273	7	-3	0	4	39.62
2.248	13	0	0	4	40.08
2.224	7	-2	2	2	40.53
2.224	1	3	1	2	40.53
2.222	15	-4	1	3	40.57
2.207	2	2	2	1	40.85
2.177	5	4	1	1	41.43
2.161	5	-3	2	1	41.76
2.159	2	-2	1	4	41.80
2.152	1	-1	1	4	41.95
2.147	4	1	2	2	42.06
2.123	3	2	1	3	42.54
2.121	5	-5	0	3	42.58
2.104	2	-4	0	4	42.96
2.100	2	-5	1	1	43.03
2.085	6	-3	1	4	43.36
2.084	1	-5	1	2	43.39
2.080	6	-3	2	2	43.46
2.066	2	0	1	4	43.79
2.048	1	4	0	2	44.19
2.019	1	-1	2	3	44.86
2.009	1	3	0	3	45.09
1.998	1	-2	2	3	45.36
1.983	4	3	2	1	45.71
1.977	17	2	2	2	45.86
1.973	1	0	2	3	45.97
1.971	2	5	0	1	46.00
1.966	1	-5	1	3	46.12
1.952	1	-4	1	4	46.48
1.937	1	-4	2	1	46.87
1.926	1	1	1	4	47.15
1.915	2	-3	2	3	47.44
1.908	9	4	1	2	47.63
1.901	8	-4	2	2	47.82
1.887	1	4	2	0	48.20
1.876	1	-1	0	5	48.49
1.876	1	3	1	3	48.49
1.872	1	2	0	4	48.60
1.871	3	1	2	3	48.61
1.845	2	5	1	1	49.35
1.841	3	-6	0	3	49.47
1.798	5	0	0	5	50.72
1.796	2	-6	1	2	50.78
1.795	1	-4	0	5	50.83

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
1.792	2	3 2 2	50.92
1.791	2	-5 1 4	50.94
1.791	2	-4 2 3	50.96
1.789	1	-2 1 5	51.01
1.787	1	-6 1 1	51.06
1.766	2	-1 1 5	51.72
1.764	9	-3 1 5	51.77
1.763	2	2 1 4	51.82
1.757	1	-2 2 4	51.99
1.753	3	-1 2 4	52.12
1.749	1	4 0 3	52.27
1.737	7	-6 1 3	52.66
1.725	1	-5 2 1	53.03
1.725	1	1 3 0	53.06
1.717	1	-3 2 4	53.31
1.716	2	-5 2 2	53.34
1.715	4	0 3 1	53.39
1.713	1	6 1 0	53.45
1.711	1	-6 0 4	53.50
1.706	4	0 2 4	53.68
1.701	1	0 1 5	53.85
1.680	1	3 0 4	54.59
1.678	1	1 3 1	54.66
1.673	4	5 2 0	54.81
1.665	1	-2 3 1	55.10
1.663	6	2 3 0	55.19
1.626	2	0 3 2	56.47
1.614	1	4 2 2	57.03
1.613	3	-2 3 2	57.04
1.612	1	-7 0 3	57.10
1.607	2	2 3 1	57.30
1.606	2	1 1 5	57.31
1.599	4	3 1 4	57.58
1.594	4	6 1 1	57.78
1.583	3	1 3 2	58.24
1.575	1	5 2 1	58.55
1.574	1	3 3 0	58.62
1.569	3	-7 1 2	58.82
1.557	2	-6 0 5	59.31
1.555	1	-1 0 6	59.38
1.553	2	7 0 0	59.45
1.544	2	-4 0 6	59.87
1.541	2	-5 2 4	59.97
1.539	1	-6 2 1	60.07
1.530	2	-1 3 3	60.48
1.524	1	-3 2 5	60.71
1.507	2	4 0 4	61.49
1.497	1	2 1 5	61.96
1.493	2	-4 3 1	62.12
1.491	2	6 2 0	62.23

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
1.489	2	7 1 0	62.29
1.483	2	0 2 5	62.60
1.476	1	-4 3 2	62.91
1.475	1	5 1 3	62.97
1.462	1	1 3 3	63.57
1.457	2	6 1 2	63.81
1.453	1	5 2 2	64.02
1.419	1	1 2 5	65.77
1.406	1	-2 3 4	66.44
1.384	1	3 1 5	67.65
1.380	1	-7 1 5	67.88
1.379	1	-7 2 1	67.89
1.376	1	-8 1 3	68.08
1.373	1	-7 2 3	68.26
1.348	1	-5 3 3	69.67
1.344	1	-4 0 7	69.94
1.339	1	7 0 2	70.23
1.338	2	-6 2 5	70.27
1.330	1	-4 2 6	70.79
1.313	2	6 2 2	71.84
1.310	2	-2 1 7	72.01
1.297	1	7 1 2	72.84
1.294	1	-1 4 1	73.04
1.287	1	-2 3 5	73.53
1.275	1	-9 0 3	74.35
1.271	1	-8 1 5	74.59
1.261	1	-8 2 2	75.32
1.252	1	-4 3 5	75.96

Structure

Hexagonal, $R\bar{3}m(166)$, Z=3. The structure was determined by Penfold and Taylor [1960].

Lattice parameters

a=9.50(1), c=4.82(1) Å [ibid.]

Density

(calculated) 2.19 g/cm^3

Thermal parameters

Isotropic [ibid.]

Atomic positions

In a disordered atomic arrangement, the 6 fluoride atoms and 12 water molecules were found to occupy one set of 36-fold positions, each site containing on the average ($\frac{1}{6}F^-$ and $\frac{1}{3}O^0$). The hydrogen positions were not determined [ibid.].

Polymorphism

Two kinds of white crystals precipitated together: the form "A", described here, and a form "B" which appeared to have a very similar structure with the c doubled [ibid.]

Scattering factors

Fe^{2+} [Thomas and Umeda, 1957]
($\frac{1}{6}F^- + \frac{1}{3}O^0$) [Berghuis et al., 1955].

Scale factor

(integrated intensities) 3.406×10^4

Additional patterns

1. PDF card 22-626[Ostrovskaya and Amirova,1969]

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
4.75	100	1 1 0	18.66
4.16	57	1 0 1	21.36
3.13	5	0 2 1	28.50
2.74	1	3 0 0	32.62
2.61	35	2 1 1	34.30
2.374	1	2 2 0	37.86
2.080	5	2 0 2	43.48
2.062	1	1 3 1	43.86
1.905	12	1 2 2	47.70
1.892	9	4 0 1	48.06
1.795	5	4 1 0	50.82
1.758	5	3 2 1	51.98
1.657	8	3 1 2	55.40
1.583	2	3 3 0	58.22
1.564	1	0 4 2	59.00
1.557	1	0 5 1	59.30
1.522	2	1 1 3	60.82
1.486	2	2 3 2	62.44
1.480	2	2 4 1	62.74
1.413	1	5 1 1	66.08
1.386	2	0 3 3	67.52
1.371	1	6 0 0	68.36
1.331	1	2 2 3	70.74
1.317	2	5 2 0	71.56
1.214	1	1 6 1	78.76
1.197	1	1 4 3	80.08
1.192	1	1 0 4	80.48
1.142	1	3 5 1	84.84

Reference

Berghuis, J., Haanapel, IJ. M., Potters, M., Loopstra, B. O., MacGillavry, C. H., and Veenendaal, A. L. (1955). Acta Cryst. **8**, 478.

Ostrovskaya, T.V., and Amirova, S.A. (1969). Zh. Neorgan. Khim. **14**, 1443. Russ. J. Inorg. Chem. (English transl.) **14**, 755.

Penfold, B.R., and Taylor, M.R.(1960). Acta Cryst. **13**, 953.

Thomas, L.H. and Umeda, K. (1957). J. Chem. Phys. **26**, 293.

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
4.75	100	1 1 0	18.67
4.16	60	1 0 1	21.35
3.13	5	0 2 1	28.50
2.74	1	3 0 0	32.63
2.61	42	2 1 1	34.29
2.375	1	2 2 0	37.85
2.079	6	2 0 2	43.48
2.062	1	1 3 1	43.86
1.905	15	1 2 2	47.70
1.892	11	4 0 1	48.05
1.795	7	4 1 0	50.81
1.758	7	3 2 1	51.99
1.657	11	3 1 2	55.40
1.583	2	3 3 0	58.22
1.565	2	0 4 2	58.99
1.557	1	0 5 1	59.29
1.522	3	1 1 3	60.81
1.486	3	2 3 2	62.45
1.480	3	2 4 1	62.74
1.413	2	5 1 1	66.08
1.386	3	0 3 3	67.51
1.371	2	6 0 0	68.35
1.331	2	2 2 3	70.74
1.317	3	5 2 0	71.56
1.307	1	4 2 2	72.25
1.302	1	4 3 1	72.53
1.214	2	1 6 1	78.75
1.197	2	1 4 3	80.09
1.192	1	1 0 4	80.49
1.142	2	3 5 1	84.84
1.128	1	3 3 3	86.16
1.019	1	5 2 3	98.25
.965	1	4 5 2	105.89
.944	1	8 1 1	109.32
.934	1	5 1 4	111.14
.926	1	4 6 1	112.55
.871	1	6 3 3	124.35
.812	1	9 1 2	143.10
.807	1	1 5 5	145.13
.799	1	9 2 1	148.96
.795	1	0 9 3	151.61
.785	1	3 4 5	157.76
.784	1	2 8 3	158.80

Lithium hydroxide hydrate, $LiOH \cdot H_2O$

Structure

Monoclinic, I2/m (12), Z=4. Pepinsky [1939] determined the structure and published his data in terms of the C2/m cell with a=7.37kX, b=8.26kX, c=3.19kX, and β=110°18'. Rabaud and Gay [1955] did further work,and Alcock [1971] refined their data to determine all the hydrogen positions.

Lattice parameters

a=6.95, b=8.28, c=3.20Å, β=95.23°.

Density

(calculated) 1.53 g/cm^3

Thermal parameters

Isotropic: hydrogen(1):B=12.3;hydrogen(2):B=14.0 [Alcock,1971]; lithium: B=3.82; oxygen(1):B=2.87 oxygen(2): B=4.67.

Atomic positions

Alcock [1971].

Scattering factors

Li^+, O^0 [International Tables, 1962]
H^0 [McWeeny, 1951]

Scale factor

(integrated intensities) 0.1301 x 10^4

Additional patterns

1. PDF card 1-1062 [Dow Chemical Co., Midland, Michigan].

Reference

Alcock, N.W. (1971). Acta Cryst. B27, 1682.
International Tables for X-ray Crystallography III 1962, pg. 202.
McWeeny, R. (1951). Acta Cryst. 4, 513.
Pepinsky, R. (1937). Z. Krist. 102A, 119.
Rabaud, H. and Gay, R. (1957). Bull. Soc. Franç. Minéral Crist. 80, 166.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				*2θ(°)* λ = 1.54056 Å
4.14	2	C	2	0		21.44
3.47	3	-2	0	0		25.68
2.97	66	0	1	1		30.02
2.80	24	1	0	1		31.94
2.66	100	-2	2	0		33.70
2.56	11	-1	3	0		34.96
2.43	45	-1	2	1		36.96
2.225	6	-3	1	0		40.50
2.167	3	2	1	1		41.64
2.086	1	C	3	1		43.34
2.070	6	0	4	0		43.70
1.958	8	-3	0	1		46.34
1.836	9	-2	3	1		49.60
1.777	3	-2	4	0		51.38
1.742	13	2	3	1		52.48
1.733	6	-4	0	0		52.78
1.664	3	1	4	1		55.14
1.646	1	3	2	1		55.80
1.611	1	-1	5	0		57.14
1.593	2	C	0	2		57.82
1.557	2	-1	1	2		59.32
1.500	2	-2	0	2		61.78
1.497	2	1	1	2		61.92
1.470	3	C	5	1		63.22
1.445	2	4	1	1		64.44
1.422	3	-3	4	1		65.58
1.380	1	C	6	0		67.86
1.374	2	-1	3	2	+	68.18
1.367	1	-5	1	0		68.58
1.353	1	-3	1	2		69.40
1.346	1	-3	5	0		69.82
1.326	1	2	2	2		71.02
1.254	1	-5	2	1	+	75.80
1.179	1	-4	2	2		81.56

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
4.14	2	0 2 0	21.45
3.47	3	-2 0 0	25.68
2.97	64	0 1 1	30.02
2.80	24	1 0 1	31.94
2.66	100	-2 2 0	33.70
2.56	11	-1 3 0	34.96
2.43	46	-1 2 1	36.96
2.225	6	-3 1 0	40.50
2.167	4	2 1 1	41.64
2.086	1	0 3 1	43.33
2.070	7	0 4 0	43.69
1.957	10	-3 0 1	46.35
1.837	11	-2 3 1	49.59
1.777	3	-2 4 0	51.37
1.742	16	2 3 1	52.49
1.733	7	-4 0 0	52.79
1.664	4	1 4 1	55.13
1.646	1	3 2 1	55.80
1.611	1	-1 5 0	57.14
1.593	3	0 0 2	57.82
1.557	2	-1 1 2	59.32
1.501	2	-2 0 2	61.77
1.498	2	1 1 2	61.91
1.469	4	0 5 1	63.23
1.445	3	4 1 1	64.45
1.422	4	-3 4 1	65.59
1.380	1	0 6 0	67.86
1.374	2	-1 3 2	68.18
1.374	1	-4 3 1	68.20
1.367	1	-5 1 0	68.58
1.353	1	-3 1 2	69.40
1.346	2	-3 5 0	69.82
1.326	2	2 2 2	71.02
1.254	1	-5 2 1	75.79
1.254	1	-1 6 1	75.81
1.239	1	-5 3 0	76.90
1.179	1	-4 2 2	81.57
1.121	1	1 5 2	86.82
1.098	1	4 5 1	89.09

Structure

Hexagonal, $R\bar{3}m$ (166), Z=3, isostructural with $CdCl_2$. The structure was determined by Pauling [1929].

Lattice parameters

a=3.632(4), c=17.795(16)Å [Ferrari et al.,]963]

Density (calculated)

3.540 g/cm^3

Thermal parameters

Isotropic, overall B=2.0

Scattering factors

Mg^{2+}, Cl^- [International Tables, 1962]

Scale factor

(integrated intensities) 1.022 x 10^4

Reference

Ferrari, A., Braibanti, A.,and Bigliardi,G.(1963). Acta Cryst. **16**, 846.

Hanawalt, J.D., Rinn, H.W., and Frevel, L.K.(1938) Ind. Eng. Chem. Anal. Ed. **10**, 457.

International Tables for X-ray Crystallography **III** (1962), pg. 202.

Pauling,L. (1929). Proc. Nat'l. Acad. Sci. USA **15**, 709.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ λ = 1.54056 Å
5.93	24	0 0 3	14.92
3.097	13	1 0 1	28.80
2.966	53	0 1 2 +	30.10
2.569	100	1 0 4	34.90
2.356	5	0 1 5	38.16
1.977	3	1 0 7 +	45.86
1.816	45	1 1 0 +	50.20
1.737	3	1 1 3	52.66
1.567	1	0 2 1	58.90
1.549	7	1 1 6 +	59.64
1.483	11	0 2 4 +	62.60
1.439	1	2 0 5 +	64.74
1.338	1	1 1 9	70.32
1.284	4	2 0 8	73.72
1.178	2	1 2 2 +	81.64
1.148	8	2 1 4 +	84.24
1.048	5	1 2 8 +	94.56
.989	1	2 1 10	102.38
.908	1	2 2 0 +	116.06
.868	1	3 1 2 +	125.04
.856	3	1 3 4 +	128.24
.812	2	3 1 8 +	143.04
.783	1	1 3 10 +	159.06

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	$2\theta(°)$ λ = 1.54056 Å
5.93	19	0 0 3	14.92
3.097	12	1 0 1	28.80
2.966	13	0 0 6	30.10
2.966	40	0 1 2	30.11
2.568	100	1 0 4	34.90
2.357	5	0 1 5	38.15
1.977	1	0 0 9	45.85
1.977	3	1 0 7	45.86
1.816	26	0 1 8	50.19
1.816	26	1 1 0	50.20
1.736	3	1 1 3	52.67
1.567	1	0 2 1	58.90
1.549	2	1 0 10	59.64
1.549	5	1 1 6	59.65
1.549	2	2 0 2	59.65
1.483	4	0 0 12	62.58
1.483	11	0 2 4	62.60
1.439	1	0 1 11	64.74
1.439	1	2 0 5	64.75
1.338	1	1 1 9	70.33
1.284	6	2 0 8	73.71
1.179	1	0 1 14	81.63
1.178	1	0 2 10	81.63
1.178	2	1 2 2	81.64
1.149	7	1 1 12	84.23
1.149	7	2 1 4	84.24
1.049	2	1 0 16	94.54
1.049	5	1 2 8	94.55
1.048	2	3 0 0	94.56
.989	1	2 1 10	102.37
.908	2	0 2 16	116.04
.908	2	2 2 0	116.06
.868	1	1 1 18	125.02
.868	1	1 2 14	125.03
.868	1	2 2 6	125.04
.868	1	3 1 2	125.05
.856	2	0 1 20	128.22
.856	2	3 0 12	128.25
.856	2	0 3 12	128.25
.856	3	1 3 4	128.26
.812	4	2 1 16	143.02
.812	4	3 1 8	143.04
.783	1	1 0 22	158.98
.783	2	1 3 10	159.06
.783	1	0 4 2	159.08

Additional patterns

1. PDF 3-0854 [Hanwalt et al., 1938]

Structure

Orthorhombic, Pcab (61), Z=16. The structure was determined by Norrestam [1967] and confirmed by Geller [1971]. The structure had previously been reported as a cubic, C-type sesquioxide [Pauling and Shappell, 1930; Swanson et al., 1960].

Lattice parameters

a=9.4161(3),b=9.4237(3), c=9.4051(3)Å (published values: 9.4157(3), 9.4233(3), 9.4047(3)Å) [Geller, 1971]

Density

(calculated) 5.026 g/cm^3

Thermal parameters

Isotropic:

Manganese(1)	B=0.335	oxygen(6)	B=0.641
Manganese(2)	B=0.416	oxygen(7)	B=0.684
Manganese(3)	B=0.577	oxygen(8)	B=0.606
Manganese(4)	B=0.584	oxygen(9)	B=0.517
Manganese(5)	B=0.573	oxygen(10)	B=0.629
		oxygen(11)	B=0.598

Atomic positions

Geller [1971]

Polymorphism

Above 35°C, α-Mn_2O_3 becomes cubic. (Substitution of less than one cation % Fe^{3+} for the Mn^{3+} ion makes the compound cubic, at room temperature.) [Geller,1971]. The alpha form described here was called β-Mn_2O_3 by Morozov and Kuznetcov [1949]. A polymorph called γ-Mn_2O_3 was prepared by dehydration of $Mn_2O_3 \cdot H_2O$, and was somewhat unstable [Verwey and deBoer, 1936].

Scattering factors

Mn^{3+} [Cromer and Waber, 1965], corrected for dispersion [Cromer, 1965].
O^{2-} [Tokonami, 1965]

Scale factor

(integrated intensities) 54.67×10^4

Additional patterns

1. PDF card 10-69 [Swanson et al., 1960].

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
4.706	1	0 0 2 +	18.84
3.844	18	1 1 2 +	23.12
3.1379	<1	2 1 2 +	28.42
2.7185	100	2 2 2	32.92
2.5157	2	3 1 2 +	35.66
2.3540	11	0 4 0 +	38.20
2.2192	<1	4 1 1 +	40.62
2.1054	<1	2 4 0 +	42.92
2.0069	9	3 3 2 +	45.14
1.9210	1	2 2 4 +	47.28
1.8462	10	3 4 1 +	49.32
1.7191	2	5 1 2 +	53.24
1.6643	27	4 4 0 +	55.14
1.6143	2	3 3 4 +	57.00
1.5686	<1	0 0 6 +	58.82
1.5272	2	1 1 6 +	60.58
1.4887	<1	6 0 2 +	62.32
1.4524	4	5 1 4 +	64.06
1.4196	11	2 6 2 +	65.72
1.3883	3	6 1 3 +	67.40
1.3589	3	4 4 4	69.06
1.3314	<1	3 5 4 +	70.70
1.3052	<1	4 6 0 +	72.34
1.2814	1	1 7 2 +	73.90
1.2802	1	2 1 7 +	73.98
1.2585	<1	6 4 2 +	75.48
1.1956	<1	5 6 1 +	80.22
1.1772	1	0 8 0 +	81.74
1.1755	1	0 0 8	81.88
1.1591	1	8 1 1 +	83.30
1.1579	1	1 1 8 +	83.40
1.1419	<1	8 2 0 +	84.84
1.1406	<1	2 0 8 +	84.96
1.1252	1	6 5 3 +	86.40
1.1097	<1	2 8 2 +	87.92
1.1087	<1	2 2 8	88.02
1.0945	<1	1 3 8 +	89.46
1.0798	2	6 6 2 +	91.02

References

Geller, S. (1971). Acta Cryst. B27, 821.
Morozov, I.S. and Kuznetcov, V.G. (1949). Izvest. Akad. Nauk. SSSR Otdel. Khim. Nauk, No. 4, 343.
Norrestam, R. (1967). Acta Chem. Scand. 21, 19.
Pauling, L. and Shappell, M. D. (1930). Z. Krist. 75, 128.
Tokonami, M. (1965). Acta Cryst. 19, 486.
Swanson,H. E., Cook,M., Isaacs,T., and Evans, E.H. (1960). Nat'l. Bur. Std. U.S. Circ.539,No.9, 37.
Verwey, E.G.W., and deBoer, J.H. (1936). Rec.trav. chim. 55, 531.

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.845	5	1 2 1	23.11
3.844	5	2 1 1	23.12
3.842	6	1 1 2	23.13
2.7179	100	2 2 2	32.93
2.3559	5	0 4 0	38.17
2.3540	5	4 0 0	38.20
2.3513	5	0 0 4	38.25
2.0078	4	3 3 2	45.12
2.0072	4	2 3 3	45.13
2.0069	4	3 2 3	45.14
1.8475	2	3 4 1	49.28
1.8471	2	4 3 1	49.29
1.8468	2	1 4 3	49.30
1.8460	2	4 1 3	49.33
1.8458	2	1 3 4	49.33
1.8454	2	3 1 4	49.34
1.6652	13	4 4 0	55.11
1.6642	13	0 4 4	55.14
1.6636	13	4 0 4	55.17
1.5286	1	1 6 1	60.52
1.5275	1	0 1 1	60.57
1.5258	1	1 1 6	60.64
1.4536	1	4 5 1	64.00
1.4533	1	5 4 1	64.01
1.4530	1	1 5 4	64.03
1.4524	1	1 4 5	64.06
1.4523	1	5 1 4	64.06
1.4519	1	4 1 5	64.08
1.4203	7	2 6 2	65.68
1.4195	7	6 2 2	65.73
1.4183	7	2 2 6	65.79
1.3892	1	3 6 1	67.35
1.3889	1	1 6 3	67.37
1.3885	1	6 3 1	67.39
1.3880	1	6 1 3	67.41
1.3873	1	1 3 6	67.46
1.3871	1	3 1 6	67.47
1.3589	4	4 4 4	69.06
1.2822	1	1 7 2	73.85
1.2814	1	7 2 1	73.90
1.2800	1	2 1 7	73.99
1.1780	1	0 8 0	81.67
1.1770	1	8 0 0	81.75
1.1756	1	0 0 8	81.87
1.1599	1	1 8 1	83.22
1.1590	1	8 1 1	83.30
1.1577	1	1 1 8	83.42
1.0804	2	6 6 2	90.95
1.0799	2	2 6 6	91.00
1.0795	2	6 2 6	91.04

Structure

Orthorhombic, Pbnm (62), Z=4. It is isostructural with goethite (α-FeOOH) and diaspore(α-AlOOH) [Gruner, 1947]. The groutite structure was determined by Collin and Lipscomb [1949] and refined by Glasser and Ingram [1968].

Lattice parameters

a=4.560, b=10.700, c=2.870(Å) [Glasser and Ingram,1968]

Density

(calculated) 4.171 g/cm^3

Thermal parameters

Isotropic [Glasser and Ingram, 1968]

Atomic positions

Glasser and Ingram [1968].

Polymorphism

MnOOH occurs also as two other minerals: manganite (γ form,monoclinic) and feitnechtite(β form, hexagonal).

Scattering factors

Mn^{3+} [International Tables, 1962]
O^{2-} [Suzuki, 1960]

Scale factor

(integrated intensities) 0.7057×10^4

Additional patterns

1. PDF card 12-733[Thompson, R.M.,Univ. of British Columbia, Vancouver, British Columbia, Canada.]

Reference

Collin, R.L. and Lipscomb, W.N.(1949). Acta Cryst. 2, 104.
Glasser, L.S.D. and Ingram, L. (1968). Acta Cryst. B24, 1233.
International Tables for X-ray Crystallography III 1962, 210.
Suzuki, T. (1960). Acta Cryst. 13, 279.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.35	9	0 2 0	16.56
4.20	100	1 1 0	21.16
3.471	10	1 2 0	25.64
2.810	34	1 3 0	31.82
2.674	29	0 4 0	33.48
2.529	13	0 2 1	35.46
2.429	4	1 0 1	36.98
2.368	48	1 1 1	37.96
2.308	17	1 4 0	39.00
2.280	2	2 0 0	39.50
2.230	2	2 1 0	40.42
2.212	7	1 2 1	40.76
2.008	5	1 3 1	45.12
1.957	3	0 4 1	46.36
1.937	4	1 5 0	46.86
1.798	3	1 4 1	50.72
1.783	2	0 6 0	51.18
1.761	9	2 1 1	51.88
1.735	6	2 4 0	52.70
1.693	26	2 2 1	54.12
1.606	18	1 5 1	57.34
1.596	7	2 3 1	57.70
1.560	3	2 5 0	59.16
1.515	9	0 6 1	61.14
1.485	1	2 4 1	62.50
1.462	4	3 2 0	63.58
1.449	4	1 7 0	64.22
1.435	6	0 0 2	64.94
1.404	1	2 6 0	66.52
1.398	3	3 3 0	66.86
1.358	3	1 1 2	69.12
1.343	3	3 0 1	69.98
1.333	1	3 1 1	70.62
1.326	1	1 2 2	71.02
1.303	1	3 2 1	72.50
1.278	4	1 3 2	74.14
1.264	3	0 4 2	75.06
1.262	3	2 6 1	75.26
1.257	2	3 3 1	75.58
1.218	1	1 4 2	78.42
1.215	1	2 0 2	78.72
1.212	2	0 8 1	78.90
1.200	3	3 4 1	79.84
1.157	1	3 6 0	83.50
1.154	3	2 8 0 +	83.78
1.133	2	4 1 0	85.62
1.106	2	2 4 2	88.30
1.078	1	3 7 0	91.24
1.073	1	3 6 1	91.76
1.070	2	2 8 1 +	92.06

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.068	3	1 9 1	92.34
1.056	1	2 5 2	93.66
1.054	1	2 9 0	93.90
1.024	1	3 2 2	97.54
1.020	2	1 7 2	98.12
1.016	1	4 3 1	98.66
1.006	1	4 5 0	99.92
1.004	1	2 6 2	100.24
1.003	1	0 10 1	100.40
1.001	2	3 3 2	100.56
.951	1	1 11 0	108.14
.948	1	3 8 1	108.72
.933	1	1 1 3	111.34
.901	1	3 6 2	117.58
.899	2	2 8 2 +	117.90
.890	2	4 1 2	119.98
.871	4	4 7 1 +	124.42
.869	2	5 0 1	124.96
.866	1	4 3 2	125.64
.862	1	3 7 2	126.70
.858	2	1 5 3 +	127.80
.856	1	2 3 3	128.20
.854	1	2 11 1	128.78
.852	1	0 12 1	129.54
.850	1	2 9 2	130.10
.843	1	0 6 3	132.04
.827	1	5 4 1	137.44
.824	1	4 5 2	138.46
.823	1	3 8 2	138.86

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
5.35	9	0 2 0	16.56
4.19	100	1 1 0	21.16
3.470	11	1 2 0	25.65
2.809	40	1 3 0	31.83
2.675	34	0 4 0	33.47
2.529	15	0 2 1	35.46
2.429	5	1 0 1	36.98
2.369	58	1 1 1	37.95
2.307	21	1 4 0	39.00
2.280	2	2 0 0	39.49
2.230	2	2 1 0	40.42
2.212	8	1 2 1	40.76
2.008	6	1 3 1	45.12
1.957	3	0 4 1	46.36
1.937	5	1 5 0	46.86
1.921	1	2 3 0	47.28
1.798	4	1 4 1	50.73
1.783	2	0 6 0	51.18
1.761	13	2 1 1	51.88
1.735	9	2 4 0	52.71
1.693	38	2 2 1	54.11
1.606	26	1 5 1	57.33
1.596	9	2 3 1	57.70
1.560	5	2 5 0	59.16
1.515	13	0 6 1	61.13
1.485	2	2 4 1	62.50
1.462	6	3 2 0	63.58
1.449	7	1 7 0	64.21
1.435	9	0 0 2	64.93
1.405	2	2 6 0	66.51
1.398	4	3 3 0	66.85
1.358	6	1 1 2	69.13
1.343	4	3 0 1	69.98
1.333	2	3 1 1	70.61
1.326	1	1 2 2	71.02
1.303	1	3 2 1	72.49
1.278	6	1 3 2	74.13
1.265	5	0 4 2	75.05
1.262	2	2 6 1	75.25
1.257	3	3 3 1	75.58
1.219	3	1 4 2	78.41
1.214	1	2 0 2	78.73
1.212	3	0 8 1	78.90
1.200	5	3 4 1	79.84
1.161	1	2 7 1	83.12
1.157	2	3 6 0	83.50
1.154	3	2 8 0	83.78
1.153	1	1 5 2	83.83
1.138	1	3 5 1	85.23
1.134	4	4 1 0	85.61

d (Å)	I	hkl	2θ(°) $\lambda = 1.54056$ Å
1.118	1	0 6 2	87.10
1.106	3	2 4 2	88.30
1.086	1	4 3 0	90.37
1.078	1	3 7 0	91.23
1.073	2	3 6 1	91.77
1.070	1	2 8 1	92.05
1.070	1	0 10 0	92.09
1.068	5	1 9 1	92.33
1.056	2	2 5 2	93.65
1.054	2	2 9 0	93.89
1.024	3	3 2 2	97.55
1.020	4	1 7 2	98.12
1.016	2	4 3 1	98.65
1.006	2	4 5 0	99.92
1.004	1	2 6 2	100.23
1.003	2	0 10 1	100.40
1.001	3	3 3 2	100.55
.979	1	1 10 1	103.75
.969	1	2 10 0	105.35
.951	2	1 11 0	108.13
.948	1	3 8 1	108.73
.942	1	0 2 3	109.76
.933	3	1 1 3	111.35
.901	2	3 6 2	117.58
.899	4	2 8 2	117.90
.899	2	5 2 0	117.92
.890	2	3 9 1	119.82
.890	5	4 1 2	119.98
.879	1	2 1 3	122.36
.871	7	4 7 1	124.40
.870	5	2 2 3	124.49
.869	2	5 0 1	124.80
.866	2	4 3 2	125.64
.862	2	3 7 2	126.71
.858	1	0 10 2	127.79
.858	5	1 5 3	127.79
.856	2	2 3 3	128.18
.854	1	2 11 1	128.79
.852	2	0 12 1	129.54
.850	3	2 9 2	130.10
.843	3	0 6 3	132.05
.837	2	3 10 1	133.96
.827	5	5 4 1	137.44
.824	4	4 5 2	138.46
.823	1	4 9 0	138.82
.823	2	3 8 2	138.87

Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (alpha HMX) $C_4H_8N_8O_8$

Structure

Orthorhombic, Fdd2 (43), Z=8. The structure was determined by Cady et al. [1963].

Lattice parameters

a=15.14, b=23.89, c=5.913Å [ibid.]

Density (calculated)

1.839 g/cm^3

Thermal parameters

Isotropic: carbon(1) B=2.731, carbon(2) B=2.641, nitrogen(1) B=2.093, nitrogen(2) B=2.374, nitrogen(3) B=2.992, nitrogen(4) B=2.900, oxygen(1) B=3.587, oxygen(2) B=4.234, oxygen(3) B=3.003, oxygen(4) B=3.658, hydrogen(3) =3.60, hydrogens (1), (2), and (4) B=0.0

Atomic positions

Erratum: in Cady et al. [op. cit.], $y_{N(1)}$ should be -0.0599 in order to derive the structure factors they give.

Polymorphism

There are 4 known polymorphic forms. The alpha modification described here is stable in the range 103 to 162 °C. [Cady, et al., 1963]

Scattering factors

C^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factor

(integrated intensities) 26.64 x 10^4

Reference

Cady, H.H., Larson, A.C., and Cromer, D.T. (1963). Acta Cryst. 16, 617.

International Tables for X-ray Crystallography III (1962). 202.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
6.39	1	2	2	0		13.84
5.97	31	0	4	0		14.82
5.37	100	1	1	1		16.50
4.53	34	1	3	1		19.58
3.79	12	4	0	0	+	23.48
3.61	45	1	5	1	+	24.64
3.52	50	2	6	0		25.26
3.46	17	3	3	1		25.74
2.986	17	0	8	0	+	29.90
2.901	7	1	7	1		30.80
2.870	11	0	2	2		31.14
2.754	34	2	0	2		32.48
2.746	23	4	6	0		32.58
2.677	5	5	1	1		33.44
2.550	4	3	7	1	+	35.16
2.501	1	2	4	2		35.88
2.469	6	6	2	0		36.36
2.391	2	1	9	1		37.58
2.373	8	0	6	2		37.88
2.325	3	6	4	0	+	38.70
2.287	13	4	2	2		39.36
2.281	8	2	10	0		39.48
2.265	3	2	6	2		39.76
2.183	4	3	9	1		41.32
2.170	3	4	4	2		41.58
2.115	1	5	7	1		42.72
2.024	1	7	1	1		44.74
2.021	2	1	11	1		44.82
1.991	1	0	12	0		45.52
1.968	1	7	3	1		46.08
1.948	3	1	1	3		46.58
1.926	2	2	12	0		47.16
1.898	2	1	3	3		47.88
1.892	2	5	9	1		48.06
1.809	1	1	5	3		50.40
1.804	1	8	4	0		50.54
1.743	1	1	13	1		52.44
1.714	1	3	5	3		53.42
1.691	1	5	11	1		54.18
1.658	1	3	13	1		55.38
1.614	3	2	12	2	+	57.02
1.580	1	8	2	2		58.36
1.540	2	8	4	2		60.02
1.484	1	7	11	1		62.56

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
6.39	1	2 2 0	13.84
5.97	30	0 4 0	14.82
5.37	100	1 1 1	16.50
4.53	35	1 3 1	19.58
3.79	4	3 1 1	23.45
3.78	10	4 0 0	23.48
3.61	48	1 5 1	24.65
3.61	3	4 2 0	24.65
3.52	56	2 6 0	25.25
3.46	18	3 3 1	25.74
2.993	4	3 5 1	29.83
2.986	18	0 8 0	29.90
2.901	8	1 7 1	30.80
2.870	13	0 2 2	31.14
2.754	40	2 0 2	32.48
2.743	8	4 6 0	32.61
2.684	1	2 2 2	33.36
2.678	5	5 1 1	33.43
2.553	1	5 3 1	35.12
2.551	4	3 7 1	35.16
2.501	1	2 4 2	35.88
2.469	7	6 2 0	36.36
2.391	3	1 9 1	37.58
2.374	10	0 6 2	37.87
2.347	4	5 5 1	38.31
2.344	1	4 8 0	38.36
2.324	4	6 4 0	38.71
2.287	17	4 2 2	39.37
2.278	3	2 10 0	39.52
2.265	3	2 6 2	39.76
2.183	5	3 9 1	41.32
2.171	4	4 4 2	41.57
2.115	1	5 7 1	42.71
2.024	1	7 1 1	44.74
2.020	1	1 11 1	44.82
1.991	2	0 12 0	45.53
1.968	1	7 3 1	46.08
1.948	4	1 1 3	46.58
1.925	2	2 12 0	47.17
1.898	2	1 3 3	47.88
1.891	2	5 9 1	48.07
1.809	1	1 5 3	50.40
1.804	1	8 4 0	50.55
1.762	1	4 12 0	51.85
1.743	1	1 13 1	52.45
1.714	2	3 5 3	53.42
1.691	1	5 11 1	54.19
1.658	1	3 13 1	55.38
1.648	1	5 1 3	55.73
1.615	2	6 8 2	56.99
1.614	1	9 1 1	57.00
1.613	2	2 12 2	57.03
1.586	1	9 3 1	58.13
1.580	1	8 2 2	58.36
1.540	3	8 4 2	60.02
1.518	1	5 13 1	60.97
1.484	1	7 11 1	62.56
1.440	1	2 2 4	64.66
1.377	1	4 0 4	68.03
1.320	1	3 17 1	71.42

Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (beta HMX) $C_4H_8N_8O_8$

Structure

Monoclinic, $P2_1/n$ (14), Z-2. The structure was determined first by Eiland and Pepinsky [1955]. Cady, Larson, and Cromer[1963] used Eiland's and Pepinsky's data and did a least squares refinement with anisotropic temperature factors, but did not determine the hydrogen positions. Choi and Boutin [1970] collected new 3-dimensional data from neutron diffraction analysis and refined parameters for all atoms including hydrogen.

Lattice parameters

a=6.54, b=11.05,c=7.37Å, β=102.8[Eiland and Pepinsky, 1955]

Density (calculated)

1.89 g/cm^3

Thermal parameters

Isotropic:hydrogen(1):B=2.892;hydrogen(2)B=2.726 hydrogen(3):B=2.790;hydrogen(4) B=3.686[Choi and Boutin,1970]. Nitrogen(1):B=1.616; nitrogen(2): B=1.468;nitrogen(3): B=1.361;nitrogen(4):B=1.676 oxygen(1):B=2.282; oxygen(2):B=2.769; oxygen(3): B=3.063; oxygen(4): B=2.523; carbon(1) B=1.294; carbon(2) B=1.600.

Atomic positions

Choi and Boutin [1970]

Polymorphism

There are 4 known polymorphic forms. The beta modification described here is the stable form at room temperature [Cady et al., 1963].

Scattering factors

H^0, O^0, N^0, C^0 [International Tables, 1962].

Scale factor

(Integrated intensities) 1.303 x 10^4

Additional patterns

1. PDF card 3-0225 [Soldate and Noyes, 1947]

Reference

Cady, H.H., Larson, A.C., and Cromer, D.T. (1963). Acta Cryst. **16**, 617.

Choi, C.S. and Boutin, H.P. (1970). Acta Cryst. B26, 1235.

Eiland, P.F. and Pepinsky, R.(1955). Z. Krist. **106**, 18.

International Tables for X-ray Crystallography III (1962), pg. 202.

Soldate, A.M. and Noyes, R.M. (1947). Anal. Chem. 19, 442.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
6.02	39	0	1	1		14.70
5.52	40	1	1	0	+	16.04
5.40	2	-1	0	1		16.40
4.85	11	-1	1	1		18.26
4.32	100	1	0	1		20.56
4.02	8	1	1	1		22.08
3.86	53	-1	2	1		23.00
3.59	1	0	0	2		24.76
3.42	7	0	1	2		26.06
3.40	23	1	2	1		26.18
3.32	9	-1	1	2		26.84
3.28	28	0	3	1		27.18
3.19	12	1	3	0	+	27.96
3.06	13	-2	1	1	+	29.12
3.04	6	-1	3	1		29.32
3.01	33	0	2	2		29.64
2.94	4	-1	2	2		30.34
2.80	77	1	3	1		31.92
2.76	7	0	4	0	+	32.38
2.70	3	-2	0	2		33.14
2.62	1	2	1	1		34.16
2.57	1	0	3	2		34.86
2.53	4	1	4	0		35.38
2.46	2	-1	4	1		36.50
2.43	7	-2	2	2	+	37.02
2.41	8	2	3	0	+	37.26
2.26	3	1	3	2		39.78
2.22	1	-1	2	3		40.56
2.197	2	0	2	3		41.04
2.190	8	0	4	2		41.18
2.178	4	-2	3	2	+	41.42
2.158	2	2	0	2		41.82
2.133	4	-3	1	1		42.34
2.119	2	-2	1	3	+	42.64
2.113	2	0	5	1		42.76
2.088	5	2	4	0	+	43.30
2.027	1	-1	3	3		44.68
2.010	3	2	2	2	+	45.06
1.984	2	3	2	0		45.70
1.958	2	1	2	3		46.32
1.926	2	3	0	1		47.16
1.913	1	-3	2	2		47.50
1.897	2	3	1	1		47.92
1.883	1	0	5	2		48.30
1.872	2	-3	3	1		48.60
1.862	3	2	3	2	+	48.86
1.842	1	0	6	0		49.44
1.817	2	-2	5	1		50.18
1.810	1	0	4	3		50.38
1.801	4	-3	0	3		50.64

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.796	4	0 0 4	50.78
1.769	1	1 6 0	51.62
1.739	1	-2 0 4	52.58
1.710	1	2 5 1	53.54
1.685	1	3 4 0	54.42
1.669	2	1 4 3	54.96
1.659	1	-2 2 4	55.34
1.627	1	-1 6 2	56.50
1.615	1	0 3 4	56.98
1.594	1	-4 0 2	57.78
1.578	1	-4 1 2	58.44
1.573	1	-2 3 4	58.64
1.550	3	1 6 2 +	59.60
1.521	1	2 6 1	60.84
1.467	1	-1 6 3	63.34

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
6.02	36	0 1 1	14.69
5.52	14	0 2 0	16.03
5.52	24	1 1 0	16.03
5.40	1	-1 0 1	16.39
4.85	11	-1 1 1	18.26
4.32	100	1 0 1	20.55
4.02	9	1 1 1	22.09
3.86	57	-1 2 1	23.00
3.59	1	0 0 2	24.76
3.42	6	0 1 2	26.05
3.40	24	1 2 1	26.17
3.32	10	-1 1 2	26.85
3.28	30	0 3 1	27.18
3.19	8	1 3 0	27.95
3.19	5	2 0 0	27.96
3.06	10	-2 1 1	29.12
3.06	4	2 1 0	29.13
3.04	5	-1 3 1	29.32
3.01	38	0 2 2	29.63
2.94	5	-1 2 2	30.34
2.80	92	1 3 1	31.91
2.76	5	0 4 0	32.38
2.76	2	2 2 0	32.39
2.70	4	-2 0 2	33.14
2.62	1	2 1 1	34.15
2.57	1	0 3 2	34.85
2.53	4	1 4 0	35.38
2.46	2	-1 4 1	36.50
2.43	2	-1 0 3	37.01
2.43	7	-2 2 2	37.01
2.41	1	-2 3 1	37.27
2.41	9	2 3 0	37.27
2.26	4	1 3 2	39.79
2.22	1	-1 2 3	40.56
2.198	2	0 2 3	41.03
2.190	9	0 4 2	41.18
2.178	4	-2 3 2	41.42
2.178	1	2 3 1	41.43
2.159	2	2 0 2	41.81
2.133	5	-3 1 1	42.34
2.119	1	-2 1 3	42.62
2.119	1	2 1 2	42.64
2.112	1	0 5 1	42.77
2.088	1	-2 4 1	43.30
2.088	4	2 4 0	43.30
2.027	1	-1 3 3	44.68
2.011	4	2 2 2	45.05
2.008	2	0 3 3	45.11
1.984	2	3 2 0	45.70
1.959	2	1 2 3	46.32
1.925	2	3 0 1	47.17
1.913	1	-3 2 2	47.50
1.897	3	3 1 1	47.92
1.882	1	0 5 2	48.31
1.872	3	-3 3 1	48.59
1.863	1	-2 3 3	48.85
1.862	3	2 3 2	48.86
1.842	2	0 6 0	49.45
1.816	1	-2 5 1	50.18
1.810	1	0 4 3	50.38
1.801	5	-3 0 3	50.65
1.797	2	0 0 4	50.77
1.769	2	1 6 0	51.61
1.743	1	-1 6 1	52.45
1.739	1	-2 0 4	52.58
1.710	1	2 5 1	53.54
1.685	1	3 4 0	54.42
1.669	3	1 4 3	54.97
1.659	1	-2 2 4	55.33
1.628	2	-1 6 2	56.49
1.615	1	0 3 4	56.98
1.594	1	-4 0 2	57.78
1.578	1	-4 1 2	58.43
1.573	1	-2 3 4	58.65
1.550	3	1 6 2	59.60
1.550	2	-3 5 1	59.61
1.522	1	2 6 1	60.83
1.467	2	-1 6 3	63.34
1.463	1	-4 3 2	63.53
1.452	1	3 5 1	64.09
1.401	2	2 6 2	66.70
1.354	1	-3 4 4	69.37

Potassium zinc bromide hydrate, $KZnBr_3 \cdot 2H_2O$

Structure
Orthorhombic, $P2_12_12_1$ (19), Z=4. The structure was determined by Holinski [1967].

Lattice parameters
a=9.327(2), b=13.067(4), c=6.786(2)Å [ibid]

Density
(calculated) 3.053 g/cm^3

Thermal parameters
Isotropic: bromine(1): B=2.86; bromine(2):B=2.97 bromine(3):B=2.86; zinc:B=2.28; potassium:B=3.51 water(1): B=2.58; water(2): B=3.31.

Atomic positions
To conform to the symmetry arrangements used in the International Tables I [1952],the values for the x parameters were replaced by -x. The value for $x_{Br(1)}$ should be -0.0129 in order to derive structure factors given by Holinski [op. cit.].

Scattering factors
O^0, K^+, Zn^{2+} [International Tables, 1962]
Br^- [Cromer and Waber, 1965]

Scale factor
(integrated intensities) 12.89 x 10^4

Reference

Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.

Holinski,R. (1967). Dissertation,Technischen Hochschule, 3392 Clausthal-Zellerfeld, W. Germany.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
7.58	6	1 1 0	11.66
6.53	18	0 2 0	13.54
6.02	14	0 1 1	14.70
5.49	47	1 0 1	16.14
5.35	11	1 2 0	16.56
5.06	13	1 1 1	17.52
4.706	21	0 2 1	18.84
4.392	1	2 1 0	20.20
4.203	4	1 2 1	21.12
3.844	32	2 0 1	23.12
3.795	2	2 2 0	23.42
3.687	5	2 1 1	24.12
3.666	4	0 3 1	24.26
3.411	63	1 3 1	26.10
3.312	5	2 2 1	26.90
3.283	13	0 1 2	27.14
3.184	100	1 0 2 +	28.00
3.097	5	1 1 2	28.80
3.089	3	1 4 0	28.88
3.023	2	3 1 0	29.52
2.944	1	0 4 1	30.34
2.882	48	2 3 1	31.00
2.826	28	3 0 1	31.64
2.763	2	3 1 1	32.38
2.743	1	2 0 2	32.62
2.685	7	2 1 2	33.34
2.676	5	2 4 0	33.46
2.595	2	3 2 1	34.54
2.573	14	1 3 2	34.84
2.489	3	2 4 1	36.06
2.371	4	3 3 1	37.92
2.360	1	1 5 1	38.10
2.321	3	2 3 2	38.76
2.292	3	3 0 2	39.28
2.285	2	1 4 2	39.40
2.252	2	3 4 0	40.00
2.205	6	4 0 1	40.90
2.198	5	1 0 3	41.02
2.178	20	0 6 0 +	41.42
2.171	12	1 1 3	41.56
2.161	3	2 5 1 +	41.76
2.138	2	3 4 1 +	42.24
2.083	1	1 2 3	43.40
2.071	1	0 5 2	43.68
2.055	10	4 3 0	44.02
2.035	10	2 0 3	44.48
2.028	30	3 3 2	44.64
2.024	20	1 6 1 +	44.74
2.008	4	0 3 3 +	45.12
2.002	3	3 5 0	45.26

d (Å)	I	hkl				2θ(°) λ = 1.54056 Å
1.967	8	4	3	1		46.10
1.963	5	1	3	3		46.22
1.943	3	2	2	3		46.70
1.919	1	3	5	1		47.34
1.901	1	4	1	2		47.80
1.895	6	2	6	1	+	47.98
1.844	11	2	3	3	+	49.38
1.833	1	0	6	2		49.70
1.828	2	4	4	1	+	49.84
1.811	1	3	1	3		50.34
1.798	14	1	6	2	+	50.72
1.767	2	1	7	1		51.68
1.758	1	4	3	2		51.96
1.740	1	4	5	0		52.56
1.734	2	5	2	1		52.74
1.725	7	3	6	1	+	53.04
1.697	5	0	0	4		54.00
1.686	2	4	5	1	+	54.38
1.682	2	0	1	4		54.50
1.669	1	1	0	4		54.98
1.663	11	5	3	1		55.20
1.658	6	4	4	2	+	55.38
1.635	2	0	7	2	+	56.20
1.624	3	4	0	3		56.64
1.611	1	1	7	2		57.14
1.609	1	1	8	0		57.20
1.606	1	2	5	3		57.32
1.588	1	0	8	1		58.04
1.579	1	3	6	2		58.40
1.575	2	5	4	1	+	58.54
1.566	1	1	8	1		58.94
1.559	1	1	3	4		59.24
1.555	3	6	0	0		59.40
1.549	3	4	6	1	+	59.62
1.530	1	5	3	2		60.44
1.521	3	4	3	3		60.84
1.518	2	5	5	0		61.00
1.497	3	2	3	4	+	61.92
1.487	3	2	6	3		62.40
1.462	1	5	4	2		63.60
1.454	1	4	4	3	+	63.98
1.431	1	6	3	1	+	65.12
1.423	1	0	5	4		65.54
1.409	1	3	3	4		66.28
1.404	2	1	9	1	+	66.56
1.386	2	2	9	0	+	67.50
1.367	2	5	3	3		68.62
1.358	1	2	9	1		69.10
1.355	1	3	4	4		69.30
1.338	3	0	6	4		70.28

Calculated Pattern *(Integrated)*

d (Å)	I	hkl			2θ(°) λ = 1.54056 Å
7.59	7	1	1	0	11.65
6.53	22	0	2	0	13.54
6.02	17	0	1	1	14.70
5.49	59	1	0	1	16.14
5.35	14	1	2	0	16.55
5.06	16	1	1	1	17.51
4.707	27	0	2	1	18.84
4.392	1	2	1	0	20.20
4.202	5	1	2	1	21.13
3.843	45	2	0	1	23.12
3.796	1	2	2	0	23.42
3.687	6	2	1	1	24.12
3.666	5	0	3	1	24.26
3.412	91	1	3	1	26.10
3.393	4	0	0	2	26.24
3.313	6	2	2	1	26.89
3.284	19	0	1	2	27.13
3.189	100	1	0	2	27.96
3.183	87	2	3	0	28.01
3.098	7	1	1	2	28.80
3.083	1	1	4	0	28.94
3.025	3	3	1	0	29.51
2.943	2	0	4	1	30.34
2.882	75	2	3	1	31.01
2.866	3	1	2	2	31.19
2.826	46	3	0	1	31.63
2.763	2	3	1	1	32.38
2.744	2	2	0	2	32.61
2.685	10	2	1	2	33.34
2.676	4	2	4	0	33.46
2.594	3	3	2	1	34.55
2.573	22	1	3	2	34.84
2.530	1	2	2	2	35.46
2.489	5	2	4	1	36.05
2.371	6	3	3	1	37.92
2.359	2	1	5	1	38.11
2.321	4	2	3	2	38.76
2.292	4	3	0	2	39.27
2.282	1	1	4	2	39.46
2.252	3	3	4	0	40.00
2.229	1	0	1	3	40.44
2.205	10	4	0	1	40.89
2.198	2	1	0	3	41.02
2.178	34	0	6	0	41.43
2.174	1	4	1	1	41.49
2.168	1	1	1	3	41.63
2.163	1	3	2	2	41.72
2.161	3	2	5	1	41.76
2.138	1	0	2	3	42.24
2.137	3	3	4	1	42.25

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.089	1	4 2 1	43.27
2.083	2	1 2 3	43.39
2.070	1	0 5 2	43.68
2.056	17	4 3 0	44.01
2.035	13	2 0 3	44.48
2.028	48	3 3 2	44.63
2.024	6	1 6 1	44.73
2.021	1	1 5 2	44.80
2.011	2	2 1 3	45.04
2.007	6	0 3 3	45.13
2.001	1	3 5 0	45.29
1.967	13	4 3 1	46.10
1.963	2	1 3 3	46.22
1.943	6	2 2 3	46.71
1.919	2	3 5 1	47.33
1.901	2	4 1 2	47.80
1.898	1	4 4 0	47.89
1.895	8	2 6 1	47.97
1.892	6	2 5 2	48.04
1.876	1	3 4 2	48.47
1.847	1	5 1 0	49.31
1.844	19	2 3 3	49.39
1.833	1	0 6 2	49.70
1.830	1	1 7 0	49.77
1.829	1	3 0 3	49.81
1.828	2	4 4 1	49.85
1.811	1	3 1 3	50.33
1.800	2	0 7 1	50.68
1.799	4	5 0 1	50.71
1.798	22	1 6 2	50.72
1.767	3	1 7 1	51.68
1.758	1	4 3 2	51.97
1.740	1	4 5 0	52.56
1.734	2	5 2 1	52.74
1.727	5	2 4 3	52.96
1.725	11	3 6 1	53.04
1.723	3	3 5 2	53.10
1.706	1	2 6 2	53.69
1.697	10	0 0 4	54.01
1.686	1	3 3 3	54.36
1.685	1	4 5 1	54.39
1.682	1	0 1 4	54.50
1.669	2	1 0 4	54.97
1.662	21	5 3 1	55.20
1.656	1	4 4 2	55.43
1.656	1	1 1 4	55.45
1.636	3	0 7 2	56.19
1.635	1	5 0 2	56.23
1.633	1	0 8 0	56.27
1.624	6	4 0 3	56.65

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.611	1	1 7 2	57.13
1.609	1	1 8 0	57.21
1.606	1	2 5 3	57.33
1.588	2	0 8 1	58.03
1.579	2	3 6 2	58.40
1.576	1	4 2 3	58.53
1.576	2	5 4 1	58.53
1.565	1	1 8 1	58.95
1.559	1	1 3 4	59.24
1.554	5	6 0 0	59.41
1.550	3	4 6 1	59.62
1.549	1	2 2 4	59.65
1.548	2	4 5 2	59.67
1.547	1	1 6 3	59.72
1.530	2	5 3 2	60.44
1.521	6	4 3 3	60.84
1.518	1	5 5 0	60.97
1.499	2	3 5 3	61.86
1.497	6	2 3 4	61.93
1.487	6	2 6 3	62.40
1.462	2	5 4 2	63.60
1.454	1	4 4 3	63.98
1.454	1	1 8 2	63.99
1.433	1	2 4 4	65.04
1.431	2	6 3 1	65.13
1.423	1	0 5 4	65.55
1.409	2	3 3 4	66.27
1.404	2	1 9 1	66.57
1.403	1	2 8 2	66.57
1.387	2	5 6 1	67.48
1.386	2	2 9 0	67.51
1.376	1	2 7 3	68.10
1.367	3	5 3 3	68.62
1.358	3	2 9 1	69.10
1.355	2	3 4 4	69.28
1.343	1	1 0 5	69.99
1.338	6	0 6 4	70.28
1.325	1	1 6 4	71.10
1.311	1	1 8 3	71.96
1.308	3	4 3 4	72.13
1.307	1	7 0 1	72.19
1.302	3	4 6 3	72.56
1.283	3	1 3 5	73.76
1.2739	1	2 8 3	74.41
1.2652	3	6 6 0	75.01
1.2485	1	2 3 5	76.19
1.2438	2	3 0 5	76.53
1.2402	5	7 0 2	76.79
1.2325	1	4 9 0	77.36
1.2291	3	6 3 3	77.62

Potassium zinc iodide hydrate, $KZnI_3 \cdot 2H_2O$

Structure

Orthorhombic, $P2_12_12_1$ (19), Z=4. The structure was determined by Holinski [private comm.,1973].

Lattice parameters

a=9.950(3), b=13.727(4), c=7.072(2)Å; published value: b=13.726 [ibid]

Density (calculated)

3.584 g/cm^3

Thermal parameters

Isotropic [Holinski, op. cit.]

Scattering factors

O^0, K^+, Zn^{2+} [International Tables, 1962]
I^- [Cromer and Waber, 1965]

Scale factor

(integrated intensities) 36.27 x 10^4

Reference

Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.

Holinski, R., Dissertation,1967; Technischen Hochschule, 3392 Clausthal-Zellerfeld, W. Germany.

International Tables for X-ray Crystallography,III 1962, pgs. 202,204.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
8.05	4	1	1	0		10.98
6.86	10	0	2	0		12.90
6.28	6	0	1	1		14.08
5.76	61	1	0	1		15.36
5.65	7	1	2	0		15.68
5.31	8	1	1	1		16.68
4.973	6	2	0	0		17.82
4.924	14	0	2	1		18.00
4.414	2	1	2	1		20.10
4.070	46	2	0	1		21.82
3.900	4	2	1	1		22.78
3.841	18	0	3	1		23.14
3.584	100	1	3	1		24.82
3.537	7	0	0	2		25.16
3.501	3	2	2	1		25.42
3.424	9	0	1	2		26.00
3.368	79	2	3	0		26.44
3.331	88	1	0	2		26.74
3.238	2	1	1	2		27.52
3.225	3	3	1	0		27.64
3.087	2	0	4	1		28.90
3.040	45	2	3	1		29.36
3.004	45	3	0	1	+	29.72
2.934	2	3	1	1		30.44
2.882	1	2	0	2		31.00
2.820	6	2	1	2	+	31.70
2.751	1	3	2	1		32.52
2.693	21	1	3	2		33.24
2.623	2	2	4	1		34.16
2.510	4	3	3	1		35.74
2.439	4	2	3	2		36.82
2.419	1	3	0	2		37.14
2.385	1	3	4	0		37.68
2.347	9	4	0	1		38.32
2.287	25	0	6	0		39.36
2.260	2	3	4	1		39.86
2.220	1	4	2	1		40.60
2.185	18	4	3	0		41.28
2.179	11	1	2	3		41.40
2.139	41	3	3	2		42.22
2.132	27	2	0	3		42.36
2.126	14	1	6	1		42.48
2.105	2	2	1	3		42.92
2.095	8	0	3	3		43.14
2.088	9	4	3	1		43.30
2.051	3	1	3	3		44.12
2.034	2	2	2	3		44.50
2.027	1	3	5	1		44.68
1.994	8	2	6	1		45.44
1.989	6	2	5	2		45.58

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.931	16	2 3 3	47.02
1.921	4	3 0 3 +	47.28
1.916	5	5 0 1	47.42
1.886	19	1 6 2	48.22
1.859	1	4 3 2	48.96
1.857	1	1 7 1	49.02
1.845	1	5 2 1	49.36
1.820	12	3 6 1	50.08
1.815	7	3 5 2	50.22
1.810	2	2 4 3	50.36
1.784	1	4 5 1	51.16
1.767	20	5 3 1 +	51.68
1.741	2	1 0 4	52.52
1.734	2	5 0 2	52.74
1.715	2	0 7 2	53.38
1.711	7	4 0 3	53.52
1.673	1	5 4 1	54.84
1.668	1	0 8 1	55.02
1.658	4	6 0 0	55.36
1.638	4	4 6 1	56.10
1.627	2	1 3 4	56.52
1.622	4	5 3 2 +	56.72
1.602	4	4 3 3	57.46
1.574	1	3 5 3	58.60
1.565	5	2 3 4	58.96
1.559	6	2 6 3	59.22
1.548	1	5 4 2	59.68
1.523	3	6 3 1	60.78
1.476	2	3 3 4	62.90
1.475	3	1 9 1	62.98
1.471	3	3 6 3	63.16
1.469	2	5 6 1	63.26
1.458	2	2 9 0	63.78
1.443	2	5 3 3	64.52
1.428	2	2 9 1	65.28
1.399	4	0 6 4 +	66.82
1.386	1	1 9 2	67.50
1.385	2	1 6 4	67.56
1.382	2	5 6 2	67.74
1.375	4	4 3 4	68.16
1.370	5	4 6 3	68.40
1.3426	3	6 6 0	70.02
1.3393	4	1 3 5	70.22
1.3330	1	7 3 1	70.60
1.3187	3	7 0 2	71.48
1.3005	5	6 3 3 +	72.64
1.2901	3	3 9 2	73.32
1.2805	1	0 9 3	73.96
1.2787	1	4 9 1	74.08
1.2401	2	2 9 3	76.80

Calculated Pattern *(Integrated)*			
d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
8.06	3	1 1 0	10.97
6.86	8	0 2 0	12.89
6.29	5	0 1 1	14.08
5.76	52	1 0 1	15.36
5.65	5	1 2 0	15.67
5.31	7	1 1 1	16.67
4.975	5	2 0 0	17.81
4.925	12	0 2 1	18.00
4.414	2	1 2 1	20.10
4.069	45	2 0 1	21.82
3.901	3	2 1 1	22.78
3.842	17	0 3 1	23.13
3.584	100	1 3 1	24.82
3.536	6	0 0 2	25.16
3.500	2	2 2 1	25.43
3.424	7	0 1 2	26.00
3.368	79	2 3 0	26.44
3.332	88	1 0 2	26.73
3.238	2	1 1 2	27.53
3.224	2	3 1 0	27.65
3.087	1	0 4 1	28.89
3.041	49	2 3 1	29.35
3.003	49	3 0 1	29.73
2.997	1	1 2 2	29.78
2.933	1	3 1 1	30.45
2.882	1	2 0 2	31.00
2.825	2	2 4 0	31.65
2.821	5	2 1 2	31.70
2.751	1	3 2 1	32.52
2.693	22	1 3 2	33.24
2.623	2	2 4 1	34.15
2.511	4	3 3 1	35.74
2.439	5	2 3 2	36.83
2.419	1	3 0 2	37.13
2.385	1	3 4 0	37.69
2.347	10	4 0 1	38.33
2.294	2	1 0 3	39.24
2.288	29	0 6 0	39.35
2.276	1	2 5 1	39.57
2.260	1	3 4 1	39.86
2.220	1	4 2 1	40.60
2.185	21	4 3 0	41.28
2.176	1	1 2 3	41.47
2.139	48	3 3 2	42.22
2.130	14	2 0 3	42.40
2.126	7	1 6 1	42.47
2.105	1	2 1 3	42.93
2.096	9	0 3 3	43.13
2.088	8	4 3 1	43.30
2.051	3	1 3 3	44.13

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.035	2	2 2 3	44.49
2.026	1	3 5 1	44.69
1.994	9	2 6 1	45.44
1.988	3	2 5 2	45.60
1.937	1	4 4 1	46.86
1.931	19	2 3 3	47.01
1.921	2	3 0 3	47.27
1.921	1	0 6 2	47.28
1.916	4	5 0 1	47.42
1.890	1	0 7 1	48.11
1.886	25	1 6 2	48.21
1.859	1	4 3 2	48.96
1.857	1	1 7 1	49.03
1.845	1	5 2 1	49.35
1.820	15	3 6 1	50.08
1.815	1	3 5 2	50.22
1.810	2	2 4 3	50.38
1.784	1	4 5 1	51.17
1.768	9	0 0 4	51.66
1.767	18	5 3 1	51.69
1.741	2	1 0 4	52.53
1.734	2	5 0 2	52.74
1.715	1	0 7 2	53.38
1.711	8	4 0 3	53.51
1.673	1	5 4 1	54.84
1.667	1	0 8 1	55.02
1.658	5	6 0 0	55.35
1.638	4	4 6 1	56.10
1.627	2	1 3 4	56.52
1.622	4	5 3 2	56.72
1.620	1	1 6 3	56.79
1.603	5	4 3 3	57.45
1.574	1	3 5 3	58.59
1.565	7	2 3 4	58.95
1.559	8	2 6 3	59.22
1.548	1	5 4 2	59.69
1.523	3	6 3 1	60.78
1.477	2	3 3 4	62.88
1.474	4	1 9 1	62.99
1.471	1	3 6 3	63.14
1.469	3	5 6 1	63.26
1.458	3	2 9 0	63.77
1.443	2	5 3 3	64.52
1.428	3	2 9 1	65.28
1.400	1	1 0 5	66.74
1.399	6	0 6 4	66.82
1.387	1	1 9 2	67.48
1.385	2	1 6 4	67.56
1.382	2	5 6 2	67.75
1.375	5	4 3 4	68.17

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.370	5	4 6 3	68.41
1.3427	4	6 6 0	70.01
1.3390	4	1 3 5	70.24
1.3331	1	7 3 1	70.59
1.3189	5	7 0 2	71.47
1.3010	3	3 0 5	72.61
1.3004	4	6 3 3	72.65
1.3003	2	4 9 0	72.66
1.2902	5	3 9 2	73.32
1.2806	1	0 9 3	73.96
1.2788	1	4 9 1	74.07
1.2401	2	2 9 3	76.80
1.2095	2	6 0 4	79.11
1.2002	1	8 3 0	79.85
1.1944	1	1 6 5	80.32
1.1932	3	5 9 1	80.41

Sodium D-tartrate hydrate, $(CHOH\text{-}CO_2Na)_2 \cdot 2H_2O$

Structure
Orthorhombic, $P2_12_12_1$ (19), Z=4. The structure was determined by Ambady and Kartha [1968].

Lattice parameters
a=11.460(5), b=14.670(5), c=4.959(3)Å [ibid.]

Density
(calculated) 1.833 g/cm^3

Thermal parameters
Anisotropic [ibid.]

Scattering factors
H^0, C^0, O^0, Na^+ [International Tables, 1962]

Scale factors
(integrated intensities) 2.400×10^4

Reference

Ambady,G.K. and Kartha,G. (1968). Acta Cryst. B24, 1540.

International Tables for X-ray Crystallography III (1962), 202.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
9.02	100	1 1 0	9.80
6.171	10	1 2 0	14.34
5.727	29	2 0 0	15.46
4.696	25	0 1 1	18.88
4.548	14	1 0 1	19.50
4.498	22	1 3 0	19.72
3.867	6	1 2 1	22.98
3.720	2	2 3 0	23.90
3.666	4	0 4 0	24.26
3.633	35	2 1 1	24.48
3.482	22	0 3 1	25.56
3.388	4	3 2 0	26.28
3.331	22	1 3 1 +	26.74
3.089	1	2 4 0	28.88
3.009	2	3 3 0	29.66
2.965	18	3 1 1	30.12
2.864	20	4 0 0	31.20
2.857	25	1 4 1	31.28
2.798	49	3 2 1	31.96
2.668	8	4 2 0	33.56
2.645	4	3 4 0	33.86
2.621	14	2 4 1	34.18
2.614	11	2 5 0	34.28
2.573	8	3 3 1	34.84
2.525	2	0 5 1	35.52
2.481	28	4 0 1 +	36.18
2.473	18	4 3 0	36.30
2.466	12	1 5 1	36.40
2.445	5	4 1 1 +	36.72
2.424	4	1 0 2	37.06
2.391	4	1 6 0	37.58
2.349	5	4 2 1 +	38.28
2.334	1	3 4 1	38.54
2.327	3	3 5 0	38.66
2.311	22	2 5 1	38.94
2.304	13	1 2 2	39.06
2.264	1	5 1 0	39.78
2.258	3	4 4 0	39.90
2.249	6	2 6 0	40.06
2.212	1	0 3 2	40.76
2.187	3	5 2 0	41.24
2.173	5	2 2 2 +	41.52
2.154	9	1 6 1	41.90
2.106	1	3 5 1	42.90
2.080	1	3 0 2	43.48
2.062	10	2 3 2 +	43.88
2.054	11	4 4 1 +	44.04
2.050	6	4 5 0	44.14
2.022	1	1 4 2	44.78
2.001	4	5 2 1 +	45.28
1.968	2	2 7 0	46.08
1.933	2	2 4 2	46.96
1.930	2	0 7 1	47.04
1.914	4	3 3 2	47.46
1.904	3	1 7 1	47.74
1.894	4	6 1 0 +	48.00
1.860	8	4 1 2 +	48.94

d (Å)	I	hkl				2θ(°) λ = 1.54056 Å
1.848	3	6	2	0		49.26
1.837	1	3	7	0		49.58
1.829	3	2	7	1		49.80
1.817	4	4	2	2		50.18
1.810	3	5	4	1		50.38
1.806	2	5	5	0		50.50
1.798	7	2	5	2		50.72
1.779	2	6	3	0		51.32
1.769	1	6	1	1		51.62
1.750	1	4	3	2		52.22
1.747	2	2	8	0		52.34
1.742	2	4	6	1		52.50
1.732	1	6	2	1		52.82
1.721	2	1	6	2		53.16
1.701	1	1	8	1		53.86
1.697	3	5	5	1	+	54.00
1.694	4	6	4	0		54.10
1.647	2	2	8	1		55.76
1.636	1	1	0	3		56.16
1.626	1	1	1	3		56.56
1.600	1	6	5	0	+	57.54
1.597	3	1	2	3	+	57.68
1.592	2	5	3	2		57.88
1.584	3	5	6	1	+	58.18
1.580	2	2	1	3		58.36
1.568	2	3	8	1		58.84
1.555	2	7	0	1		59.40
1.551	3	1	3	3		59.54
1.547	2	7	1	1	+	59.72
1.542	1	2	7	2		59.94
1.517	1	3	0	3		61.02
1.513	1	6	0	2		61.20
1.511	3	2	3	3	+	61.32
1.505	2	6	1	2		61.56
1.495	1	7	4	0		62.04
1.488	1	4	6	2		62.36
1.486	1	3	2	3		62.46
1.482	2	7	3	1	+	62.64
1.477	1	5	7	1		62.88
1.467	1	0	10	0		63.34
1.432	1	7	4	1	+	65.10
1.428	2	2	8	2	+	65.28
1.417	1	4	9	0		65.86
1.412	1	6	7	0		66.14
1.370	1	8	1	1		68.42
1.227	1	6	7	2		77.78
1.222	1	0	2	4		78.12
1.220	1	5	5	3		78.34
1.175	1	0	11	2		81.96

Calculated Pattern *(Integrated)*

d (Å)	I	hkl			2θ(°) λ = 1.54056 Å
9.03	100	1	1	0	9.79
6.178	11	1	2	0	14.32
5.730	32	2	0	0	15.45
4.698	28	0	1	1	18.87
4.551	15	1	0	1	19.49
4.516	4	2	2	0	19.64
4.498	24	1	3	0	19.72
3.867	7	1	2	1	22.98
3.720	2	2	3	0	23.90
3.667	4	0	4	0	24.25
3.633	44	2	1	1	24.48
3.482	27	0	3	1	25.56
3.388	5	3	2	0	26.28
3.339	13	2	2	1	26.68
3.332	19	1	3	1	26.74
3.089	1	2	4	0	28.88
3.010	2	3	3	0	29.65
2.964	25	3	1	1	30.13
2.865	24	4	0	0	31.19
2.856	24	1	4	1	31.30
2.797	68	3	2	1	31.97
2.669	11	4	2	0	33.55
2.646	5	3	4	0	33.85
2.622	20	2	4	1	34.17
2.612	8	2	5	0	34.31
2.573	11	3	3	1	34.84
2.525	2	0	5	1	35.52
2.481	36	4	0	1	36.18
2.479	3	0	0	2	36.20
2.472	5	4	3	0	36.31
2.466	11	1	5	1	36.40
2.446	4	4	1	1	36.71
2.445	2	0	6	0	36.73
2.423	5	1	0	2	37.07
2.391	6	1	6	0	37.58
2.350	7	4	2	1	38.27
2.349	1	0	2	2	38.29
2.334	1	3	4	1	38.54
2.327	3	3	5	0	38.66
2.311	32	2	5	1	38.94
2.301	2	1	2	2	39.11
2.265	1	5	1	0	39.77
2.258	4	4	4	0	39.90
2.249	7	2	6	0	40.06
2.211	1	0	3	2	40.77
2.193	1	0	6	1	41.13
2.188	4	5	2	0	41.23
2.173	6	2	2	2	41.51
2.171	3	1	3	2	41.55
2.154	13	1	6	1	41.91

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
2.106	1	3 5 1	42.90
2.080	1	3 0 2	43.48
2.063	8	2 3 2	43.85
2.062	7	1 7 0	43.88
2.060	2	5 1 1	43.92
2.059	2	3 1 2	43.93
2.055	8	4 4 1	44.03
2.054	3	0 4 2	44.05
2.050	2	4 5 0	44.14
2.022	2	1 4 2	44.79
2.002	3	5 2 1	45.27
2.001	3	3 2 2	45.28
1.968	3	2 7 0	46.08
1.934	3	2 4 2	46.95
1.930	2	0 7 1	47.03
1.914	6	3 3 2	47.47
1.904	4	1 7 1	47.74
1.894	5	6 1 0	47.99
1.894	1	0 5 2	48.00
1.860	2	4 6 0	48.93
1.860	11	4 1 2	48.94
1.848	4	6 2 0	49.26
1.837	1	3 7 0	49.57
1.829	4	2 7 1	49.80
1.816	7	4 2 2	50.18
1.810	3	5 4 1	50.38
1.806	1	5 5 0	50.49
1.798	12	2 5 2	50.73
1.779	3	6 3 0	51.31
1.769	2	6 1 1	51.61
1.751	1	4 3 2	52.21
1.746	3	2 8 0	52.34
1.741	2	4 6 1	52.51
1.732	1	6 2 1	52.81
1.721	3	1 6 2	53.17
1.701	1	1 8 1	53.86
1.697	2	5 5 1	53.98
1.697	2	3 5 2	54.00
1.694	5	6 4 0	54.09
1.675	1	6 3 1	54.77
1.647	4	2 8 1	55.76
1.636	1	1 0 3	56.17
1.626	2	1 1 3	56.55
1.601	1	4 7 1	57.52
1.601	1	6 5 0	57.53
1.598	2	7 2 0	57.64
1.597	3	1 2 3	57.68
1.591	2	5 3 2	57.90
1.585	2	5 6 1	58.17
1.584	2	3 6 2	58.19

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
1.579	1	2 1 3	58.40
1.568	2	3 8 1	58.83
1.555	3	7 0 1	59.40
1.552	4	1 3 3	59.53
1.548	1	0 9 1	59.66
1.547	1	5 7 0	59.74
1.546	1	7 1 1	59.77
1.542	1	2 7 2	59.96
1.523	1	6 5 1	60.75
1.517	1	3 0 3	61.03
1.513	1	6 0 2	61.20
1.511	4	2 3 3	61.32
1.509	1	3 1 3	61.39
1.505	1	6 1 2	61.56
1.495	2	7 4 0	62.03
1.488	2	4 6 2	62.36
1.486	1	3 2 3	62.46
1.482	1	6 2 2	62.64
1.482	1	7 3 1	62.65
1.476	1	5 7 1	62.89
1.467	2	0 10 0	63.35
1.460	1	5 5 2	63.69
1.432	1	5 8 0	65.09
1.431	1	7 4 1	65.12
1.430	1	7 5 0	65.20
1.429	1	1 5 3	65.24
1.428	1	2 8 2	65.30
1.417	1	4 9 0	65.87
1.412	1	6 7 0	66.14
1.370	1	8 1 1	68.41
1.362	1	0 9 2	68.88
1.353	1	8 2 1	69.43
1.348	1	3 5 3	69.72
1.227	1	6 7 2	77.79
1.222	1	0 2 4	78.12
1.219	1	5 5 3	78.35
1.175	1	0 11 2	81.96

Structure

Orthorhombic, Pnam (62), Z=4. The structure was determined by Mumme and Wadsley (1968).

Lattice parameters

a=10.35(1), b=11.25(1), c=3.70(1)Å [ibid.]

Density (calculated)

4.713 g/cm^3

Thermal parameters

Isotropic [ibid.]

Scattering factors

O^{2-} [Suzuki, 1960]
Y^{3+}, Ti^{4+} [Cromer and Waber,1965]. These factors were corrected for dispersion [Cromer, 1965].

Scale factors

(integrated intensities) 10.05×10^4

Additional patterns

1. PDF card 21-1464 [Garton and Wanklyn, 1968]

Reference

Cromer, D.T. (1965). Acta Cryst. 18, 17.

Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.

Garton, G. and Wanklyn, B.M. (1968). J. Mater.Sci. 3, 395.

Mumme, W.G. and Wadsley, A.D. (1968). Acta Cryst. B24, 1327.

Suzuki, T. (1960). Acta Cryst. 13, 279.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
7.61	18	1 1 0	11.62
5.63	2	0 2 0	15.74
5.18	11	2 0 0	17.12
4.94	3	1 2 0	17.94
4.70	6	2 1 0	18.86
3.81	2	2 2 0	23.34
3.53	24	1 3 0 +	25.24
3.33	2	1 1 1	26.76
3.04	74	2 3 0	29.40
3.01	100	2 0 1	29.66
2.94	9	3 2 0	30.36
2.91	4	2 1 1	30.72
2.71	2	1 4 0	32.98
2.63	25	0 3 1	34.02
2.587	8	4 0 0	34.64
2.552	9	1 3 1	35.14
2.539	8	3 3 0	35.32
2.521	4	4 1 0	35.58
2.462	3	3 1 1	36.46
2.302	7	3 2 1	39.10
2.198	4	1 5 0	41.02
2.130	1	4 3 0	42.40
2.121	2	4 0 1	42.60
2.093	8	3 3 1	43.18
2.084	4	4 1 1	43.38
2.055	3	2 4 1	44.02
2.036	2	5 1 0	44.46
1.984	3	4 2 1	45.68
1.943	1	5 2 0	46.72
1.904	3	4 4 0	47.72
1.890	1	1 5 1	48.10
1.875	4	0 6 0	48.52
1.850	23	0 0 2	49.22
1.845	55	4 3 1 +	49.34
1.798	1	1 1 2	50.74
1.783	2	5 1 1	51.18
1.720	6	5 2 1	53.20
1.705	1	6 1 0	53.72
1.693	1	4 4 1	54.12
1.679	2	3 5 1	54.60
1.667	1	5 4 0	55.04
1.651	10	1 6 1 +	55.62
1.647	7	3 6 0	55.76
1.638	4	1 3 2	56.10
1.627	4	5 3 1	56.50
1.591	5	2 6 1	57.90
1.580	15	2 3 2	58.36
1.567	5	6 3 0 +	58.88
1.563	7	6 0 1	59.04
1.549	2	6 1 1	59.66
1.524	1	5 5 0	60.74
1.519	2	4 6 0	60.96
1.505	10	3 6 1 +	61.58
1.495	2	3 3 2	62.02
1.492	2	4 1 2	62.18
1.470	1	6 4 0	63.18
1.466	2	7 1 0	63.38
1.443	1	6 3 1	64.52
1.430	1	7 2 0	65.18
1.418	1	2 7 1	65.82
1.415	1	1 5 2	65.94

d (Å)	I	hkl				2θ(°) λ = 1.54056 Å
1.390	2	5	6	0		67.32
1.369	1	5	1	2		68.48
1.367	2	6	4	1		68.62
1.363	1	7	1	1		68.82
1.327	1	4	4	2		70.98
1.317	1	0	6	2		71.60
1.306	6	1	6	2		72.26
1.294	1	8	0	0		73.08
1.285	1	8	1	0		73.64
1.281	1	4	7	1		73.94
1.241	1	1	9	0		76.74
1.234	1	7	4	1		77.26
1.230	1	3	6	2	+	77.52
1.200	4	2	0	3	+	79.88
1.196	3	6	3	2		80.20
1.193	2	8	2	1		80.44
1.176	4	1	9	1	+	81.88
1.174	4	4	6	2		82.04
1.172	4	0	3	3	+	82.20
1.164	1	1	3	3		82.86
1.161	1	8	3	1		83.12
1.151	1	6	4	2		84.00
1.149	1	7	1	2		84.20
1.131	1	7	2	2		85.82
1.120	2	3	9	1		86.90
1.111	2	5	6	2		87.78
1.109	2	5	8	1	+	87.94
1.108	2	7	6	1		88.10
1.104	1	7	3	2		88.50
1.093	1	9	1	1		89.62
1.070	1	5	9	0		92.08
1.067	3	4	3	3		92.40
1.060	1	8	0	2		93.20
1.055	1	8	1	2		93.74
1.044	1	7	7	1		95.10
1.041	1	5	2	3		95.42
1.031	2	1	9	2		96.74
1.028	3	5	9	1		97.08
1.025	3	1	6	3		97.40
1.020	1	5	3	3		98.14
1.011	1	2	6	3		99.32
1.003	1	6	0	3		100.30
.992	3	3	9	2	+	101.88
.987	2	3	6	3		102.56
.972	1	8	7	1		104.78
.939	1	10	4	1		110.16
.934	1	1	12	0		111.18
.926	1	5	9	2		112.54
.925	1	0	0	4		112.76
.923	2	8	6	2	+	113.20
.911	1	10	5	1		115.40

Calculated Pattern *(Integrated)*					
d (Å)	I	hkl			2θ(°) λ = 1.54056 Å
7.62	14	1	1	0	11.61
5.63	2	0	2	0	15.74
5.18	10	2	0	0	17.12
4.94	2	1	2	0	17.93
4.70	5	2	1	0	18.86
3.81	2	2	2	0	23.34
3.53	24	1	3	0	25.24
3.51	1	0	1	1	25.32
3.33	2	1	1	1	26.76
3.04	78	2	3	0	29.39
3.01	100	2	0	1	29.66
2.94	9	3	2	0	30.37
2.91	4	2	1	1	30.72
2.71	2	1	4	0	32.98
2.63	27	0	3	1	34.01
2.588	8	4	0	0	34.64
2.552	10	1	3	1	35.13
2.539	8	3	3	0	35.32
2.522	4	4	1	0	35.57
2.462	3	3	1	1	36.46
2.302	8	3	2	1	39.09
2.199	4	1	5	0	41.02
2.188	1	1	4	1	41.22
2.130	1	4	3	0	42.41
2.120	2	4	0	1	42.60
2.093	9	3	3	1	43.18
2.084	4	4	1	1	43.39
2.055	3	2	4	1	44.03
2.036	2	5	1	0	44.46
1.984	4	4	2	1	45.69
1.943	1	5	2	0	46.72
1.904	3	4	4	0	47.72
1.890	1	1	5	1	48.10
1.878	2	3	4	1	48.42
1.875	4	0	6	0	48.51
1.850	22	0	0	2	49.21
1.846	43	4	3	1	49.33
1.845	16	1	6	0	49.35
1.798	1	1	1	2	50.74
1.784	2	5	1	1	51.17
1.720	7	5	2	1	53.21
1.705	2	6	1	0	53.71
1.693	2	4	4	1	54.12
1.679	3	3	5	1	54.60
1.667	1	5	4	0	55.04
1.651	13	1	6	1	55.62
1.649	1	6	2	0	55.69
1.647	1	3	6	0	55.75
1.638	4	1	3	2	56.10
1.627	5	5	3	1	56.50

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.591	6	2 6 1	57.90
1.580	20	2 3 2	58.36
1.567	5	6 3 0	58.88
1.566	2	3 2 2	58.93
1.563	7	6 0 1	59.03
1.549	3	6 1 1	59.66
1.523	2	5 5 0	60.75
1.518	2	4 6 0	60.97
1.505	9	3 6 1	61.57
1.505	4	4 0 2	61.57
1.495	3	3 3 2	62.02
1.492	1	4 1 2	62.18
1.474	1	0 7 1	63.01
1.470	2	6 4 0	63.18
1.466	2	7 1 0	63.40
1.443	1	6 3 1	64.52
1.430	2	7 2 0	65.18
1.418	1	2 7 1	65.82
1.416	2	1 5 2	65.93
1.390	2	5 6 0	67.32
1.376	1	7 3 0	68.11
1.369	1	5 1 2	68.47
1.367	2	6 4 1	68.62
1.363	1	7 1 1	68.83
1.327	2	4 4 2	70.97
1.317	2	0 6 2	71.59
1.306	9	1 6 2	72.26
1.301	1	5 6 1	72.61
1.294	2	8 0 0	73.08
1.285	1	8 1 0	73.64
1.281	1	4 7 1	73.94
1.254	1	6 1 2	75.81
1.241	2	1 9 0	76.73
1.234	1	7 4 1	77.26
1.231	1	6 2 2	77.47
1.230	1	3 6 2	77.52
1.214	1	8 1 1	78.76
1.201	2	6 6 1	79.81
1.200	5	2 0 3	79.89
1.196	4	6 3 2	80.21
1.193	1	8 2 1	80.40
1.177	4	1 9 1	81.79
1.176	1	5 5 2	81.84
1.176	1	6 7 0	81.85
1.175	1	8 4 0	81.89
1.175	3	3 9 0	81.90
1.174	2	4 6 2	82.04
1.172	2	7 5 1	82.18
1.172	3	0 3 3	82.21
1.164	1	1 3 3	82.85

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.161	2	8 3 1	83.11
1.151	1	6 4 2	84.00
1.149	1	7 1 2	84.20
1.131	1	7 2 2	85.82
1.120	3	3 9 1	86.90
1.111	2	5 6 2	87.78
1.110	1	5 8 1	87.92
1.109	1	3 3 3	87.95
1.108	2	7 6 1	88.11
1.104	1	7 3 2	88.51
1.093	1	9 1 1	89.62
1.078	1	9 2 1	91.23
1.070	1	5 9 0	92.09
1.067	6	4 3 3	92.39
1.060	2	8 0 2	93.19
1.056	1	8 1 2	93.73
1.044	1	7 7 1	95.10
1.041	1	5 2 3	95.43
1.031	2	1 9 2	96.73
1.028	4	5 9 1	97.07
1.025	3	1 6 3	97.40
1.024	1	9 5 0	97.57
1.020	1	5 3 3	98.13
1.011	1	2 6 3	99.32
1.003	2	6 0 3	100.31
.993	1	10 1 1	101.76
.992	1	6 7 2	101.83
.992	1	8 4 2	101.87
.992	4	3 9 2	101.88
.987	3	3 6 3	102.55
.972	2	8 7 1	104.78
.962	1	9 2 2	106.35
.959	1	8 5 2	106.86
.955	1	5 10 1	107.53
.955	1	7 9 0	107.59
.945	1	6 4 3	109.20
.939	2	10 4 1	110.15
.934	1	1 12 0	111.18
.926	1	5 9 2	112.53
.925	2	0 0 4	112.76
.923	1	8 6 2	113.16
.923	1	9 4 2	113.21
.911	2	10 5 1	115.39

CUMULATIVE INORGANIC INDEX

[5] Further work on this program is in progress, and it is anticipated that additional sections will be issued. Therefore, the accumulative index here is not necessarily the concluding index for the project.

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CUMULATIVE ORGANIC INDEX

CUMULATIVE MINERAL INDEX

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* Natural mineral.
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Standard x-ray diffraction patterns are presented for 70 substances. Fifty-two of these patterns represent experimental data and 18 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The denisities and lattice constants were calculated, and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

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